PB81-217648

Evaluation of Relative Environmental Hazards from a Coal Gasifier

Research Triangle Inst.
Research Triangle Park, NC

Prepared for

Industrial Environmental Research Lab.
Research Triangle Park, NC

Jun 81

U.S. Department of Commerce
National Technical Information Service
NTIS

EPA-600/7-81-100
June 1981
PB81-217648

RTI/1934/00-02F

EVALUATION OF RELATIVE ENVIRONMENTAL HAZARDS FROM A COAL GASIFIER

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EPA Cooperative Agreement No. CR804979

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Research Triangle Park, NC 27711

Prepared for

U.S. ENVIRONMENTAL PROTECTION AGENCY
OFFICE OF RESEARCH AND DEVELOPMENT
WASHINGTON, DC 20460

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PAGE NUMBER
EPA-287 (Cin.)
(4-78)

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-600/7-81-100	2.	3. RECIPIENT'S ACCESSION NO. PB81 217648
4. TITLE AND SUBTITLE Evaluation of Relative Environmental Hazards from a Coal Gasifier		5. REPORT DATE June 1981
		6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) S. K. Gangwal, J. G. Cleland, and R. S. Truesdale		8. PERFORMING ORGANIZATION REPORT NO. RTI/1934/00-02F
9. PERFORMING ORGANIZATION NAME AND ADDRESS Research Triangle Institute P.O. Box 12194 Research Triangle Park, North Carolina 27709		10. PROGRAM ELEMENT NO. CCZN1A
		11. CONTRACT/GRANT NO. Cooperative Agreement CR804979
12. SPONSORING AGENCY NAME AND ADDRESS EPA, Office of Research and Development Industrial Environmental Research Laboratory Research Triangle Park, NC 27711		13. TYPE OF REPORT AND PERIOD COVERED Final; 11/76 - 4/81
		14. SPONSORING AGENCY CODE EPA/600/13

15. SUPPLEMENTARY NOTES IERL-RTP project officer is N. Dean Smith, Mail Drop 61, 919/541-2708.

16. ABSTRACT The report gives results of an evaluation of relative environmental hazards from a laboratory-scale coal gasifier. Detailed chemical analyses of four effluent streams (gas, aqueous condensate, tar, and ash) were performed for more than 30 gasification runs on a variety of coals, from lignite to bituminous. It briefly describes the gasification reactor, the associated sampling and analysis system, problems encountered with analyses, and special techniques for analyzing complex samples. Relative environmental hazards were determined using the Multimedia Environmental Goals methodology. Toxicity and mutagenicity were assessed using bioassay data. More than 400 effluent stream constituents were identified. Environmentally, the most significant effluent stream is aqueous condensate, followed by tar, product gas, and ash. However, on an equivalent weight basis, the tar stream is more toxic and mutagenic than aqueous condensate. Polycyclic aromatic hydrocarbons and organic bases are the most mutagenic fractions of the tar. Coal pyrolysis and gasification at higher temperatures leads to reduced tar mutagenicity. The most environmental significant constituents (by stream) are: (1) product gas--CO, benzene, H2S, and carbonyl sulfide; (2) aqueous condensate--phenol/cresols/xylenols (PCX), NH3, sulfides, thiocyanates, CN, As, and chlorides; and (3) ash--As, Ni, Be, and Se.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS		b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group	
Pollution	Analyzing	Pollution Control	13B	14B
Coal Gasification		Stationary Sources	13H	
Coal		Hazards	08G, 21D	
Toxicity			06T	
Mutagens			06E	
Chemical Analysis			07D	

18. DISTRIBUTION STATEMENT Release to Public	19. SECURITY CLASS (This Report) Unclassified	21. NO. OF PAGES 108
	20. SECURITY CLASS (This page) Unclassified	22. PRICE

EPA Form 2220-1 (9-73)

EVALUATION OF RELATIVE ENVIRONMENTAL HAZARDS FROM A COAL GASIFIER

ABSTRACT

During the past four years, a laboratory-scale coal gasification facility was developed and used to study the generation, evaluation, and environmental assessment of pollutants from coal gasification operation. Detailed chemical analyses of the four effluent streams namely gas, aqueous condensate, tar, and ash were performed for more than 30 runs in which a variety of coals ranging from lignite to bituminous were gasified.

Brief descriptions are given for the gasification reactor and the associated sampling and analysis system. Problems encountered with analysis and special techniques for analysis of complex samples are described. The relative environmental hazards of the various effluent streams is determined, using multimedia environmental goals (MEG) methodology. Toxicity and mutagenicity of the streams are assessed using bioassay.

More than 400 constituents are identified in the various effluent streams. Environmentally significant and nonsignificant constituents are ranked according to discharge severity. The nonsignificant constituents are candidates for elimination in future research. Finally, data from the laboratory gasifier are discussed in relation to those reported on large scale processes.

TABLE OF CONTENTS

Abstract ii
Figures iv
Tables vi
Acknowledgments viii
1.0 INTRODUCTION 1
2.0 REACTOR, SAMPLING, AND ANALYSIS SYSTEMS 3
 2.1 REACTOR SYSTEM 3
 2.2 SAMPLING SYSTEM 7
 2.3 ANALYTICAL SYSTEM 7
 2.4 PROBLEMS 10
3.0 SPECIAL ANALYTICAL TECHNIQUES 12
 3.1 PCX IN CONDENSATE BY HPLC/LOW WAVELENGTH UV 12
 3.2 GLASS CAPILLARY GAS CHROMATOGRAPHY (GC^2) 12
4.0 MEG METHODOLOGY AND BIOASSAY 17
 4.1 MEG METHODOLOGY 17
 4.2 BIOASSAY 18
5.0 RESULTS 20
 5.1 STREAM CONCENTRATIONS 20
 5.2 PRODUCTION FACTORS AND CONTROL PRIORITIES 34
 5.3 TOTAL STREAM EVALUATION 44
 5.4 BIOASSAY RESULTS 50
6.0 DISCUSSION 58
 6.1 OVERALL STREAM COMPARISONS 58
 6.2 PRODUCT GAS 58
 6.3 AQUEOUS CONDENSATE 60
 6.4 TAR 71
 6.5 ASH 75
7.0 CONCLUSIONS 87
References 89
Glossary 97

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

FIGURES

Number Page

1 Coal gasification: influent and effluent streams 4
2 Laboratory gasifier and sampling system at RTI 6
3 Samples collected during gasification of coal 8
4 Analytical program 9
5 FID chromatogram of crude tar from gasification of Wyoming coal (Run C2) 14
6 FPD chromatogram of crude tar from gasification of a mixture of Illinois No.6 coal and limestone (Run C6) 15
7 NPD chromatogram of tar from gasification of a mixture of Illinois No.6 coal and $CaCO_3$ (Run C6) 16
8 Ranges of concentrations for most significant product gas constituents 35
9 Ranges of concentrations for product gas constituents of medium significance 36
10 Ranges of concentrations for significant aqueous condensate constituents 37
11 Ranges of concentrations for significant tar constituents . . 38
12 Ranges of concentrations for significant ash elements 39
13 Ranges of production factors for significant product gas constituents 40
14 Ranges of production factors for significant aqueous condensate constituents 41
15 Ranges of production factors for significant tar constituents 42
16 Ranges of production factors for significant ash elements . . 43
17 Ranges of control priorities for significant product gas constituents 45
18 Ranges of control priorities for significant aqueous condensate constituents 46
19 Ranges of control priorities for significant tar constituents 47
20 Ranges of control priorities for significant ash elements . . 48
21 Ranges of tar partition fractions as weight percent of crude tar 53
22 Comparison of mutagenicities for Wyoming semibatch tar and its fractions to those for Wyoming continuous tar and its fractions 54

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

LIST OF FIGURES (continued).

Number Page

23 Comparison of mutagenicities for North Dakota semibatch tar and its fractions to those for North Dakota continuous tar and its fractions 55

24 Mutagenicities for Illinois semibatch and continuous tars and semibatch tar fractions 56

25 Aqueous condensate pollutant production from gasification of Illinois No.6 coal 68

EPA-287 (Cin.)
(4-76)

TABLES

Number Page

1 Analysis of Fuels Gasified at RTI 5
2 Product Gas Constituents Eliminated Based on Maximum Concentration 21
3 Aqueous Condensate Constituents Eliminated Based on Maximum Concentration 22
4 Tar Constituents Eliminated Based on Maximum Concentration . . 23
5 Ash Elements Eliminated Based on Maximum Concentration 24
6 Product Gas Constituents Not Eliminated Based on Maximum Concentration 25
7 Aqueous Condensate Constituents Not Eliminated Based on Maximum Concentration 26
8 Tar Constituents Not Eliminated Based on Maximum Concentration 27
9 Ash Elements Not Eliminated Based on Maximum Concentration . . 28
10 Product Gas Constituents Ranked on the Basis of Discharge Severity: (Mean Concentration/DMEG) 30
11 Aqueous Condensate Constituents Ranked on the Basis of Discharge Severity: (Mean Concentration/DMEG) 31
12 Tar Constituents Ranked on the Basis of Discharge Severity: (Mean Concentration/DMEG) 32
13 Ash Elements Ranked on the Basis of Discharge Severity: (Mean Concentration/DMEG) 33
14 Gross Effluent Stream Amounts Per Unit of Coal 49
15 Overall Stream Evaluation Based on Mean Pollutant Concentrations 51
16 Comparison of Effluent Stream Production from Different Gasifiers 59
17 Comparison of Concentrations [$\mu g/m^3$] and Production Factors [$\mu g/g$ coal]$^+$ of Significant Product Gas Constituents from Different Gasifiers 61
18 Comparison of Concentration of Significant Product Gas Constituents with Combustion Flue Gas and Particulates, Ambient Background Concentration, and NIOSH-Recommended Exposure Limit 63
19 Comparison of Concentration [$\mu g/L$] and Production Factors$^+$ [$\mu g/g$ coal] of Significant Aqueous Condensate Constituents from Different Gasifiers 65

BEGIN LAST LINE OF TEXT
BOTTOM OF IMAGE AREA OUTSIDE DIMENSION FOR TABLES AND ILLUSTRATIONS
3/8"
PAGE NUMBER

EPA-287 (Cin.)
(4-76)

LIST OF TABLES (continued).

Number — Page

20 Comparisons of Concentrations [μg/L] of Significant Aqueous Constituents with Concentrations in Effluents from Other Coal Conversion Processes, Ambient Levels, and Regulated Levels . . . 69
21 PNA Compounds Detected in the Aqueous Condensate from the Gasification of North Dakota Lignite (Test 43) 72
22 Comparison of RTI Tar Composition and Production to those from Other Gasifiers 74
23 Tar Composition for Various Processes (%) 76
24 Comparison of Concentrations [μg/g] of Coal Gasification Tar Constituents with Coal Liquids, Asphalt, Pitch and Combustion Particulates 77
25 Comparisons of Concentrations [μg/g] of Significant Ash Constituents from Different Gasifiers 80
26 Comparisons of Concentrations [μg/g] of Significant Trace Elements in RTI Gasifier Ash with Combustion Ash, Coal, and A Typical Shale 82
27 Maximum Concentrations of Contaminants for Characteristic EP Toxicity 84

EPA-287 (Cin.)
(4-75)

ACKNOWLEDGMENTS

The work reported herein was carried out as part of a project entitled "Pollutants from Synthetic Fuels Production" under sponsorship of the Fuel Process Branch, Industrial Environmental Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, N.C. The guidance of Dr. N. Dean Smith, Project Officer, Mr. William J. Rhodes, Program Manager, and Mr. T. Kelly Janes, Branch Chief, are acknowledged.

The substantial contributions of several staff members, especially Forest O. Mixon, William J. McMichael, Duane G. Nichols, David Green, Keith Leese, Joel Everett, Peter Grohse, David Hardison, Charles Sparacino, Alan Kolber, and Ruth Zweidinger were invaluable for completion of this project.

PAGE NUMBER
EPA-287 (Cin.)
(4-76)

1.0 INTRODUCTION

The Research Triangle Institute (RTI), under sponsorship of the U.S. Environmental Protection Agency (EPA), undertook a research project to study pollution problems associated with coal gasification processes. The primary objectives of this research were to perform a detailed characterization of pollutants in various coal gasification effluent streams, to understand the relationship of gasification operating conditions to pollutant production, and to identify environmentally significant and nonsignificant effluent streams and their constituents in order to obtain future directions for research in the assessment of potential environmental control techniques.

During the four years of this project, four major reports were issued. In these reports, the construction and preliminary testing operations on a laboratory-scale coal gasification facility,[1] sampling and analytical techniques,[2] screening test results,[3] and environmental evaluation of screening tests[4] were described.

In this report, first a brief description of the reactor, sampling, and analysis systems is given with special emphasis on problems encountered and recent modifications. Then, effluent stream results from analytical and bioassay testing are presented for some 33 important gasification tests. Using the multimedia environmental goals methodology,[5-8] these results are then analyzed to identify the environmentally significant as well as nonsignificant effluent streams and their constituents. The results are discussed in detail in relation to those obtained on larger scale units. Finally, based on problems encountered in reactor operations, measurement techniques and data analysis, directions for future research are identified.

The emphasis in the report is to evaluate the ranges of pollutant production under a variety of process conditions, primarily to determine their environmental (health) impact rather than to determine the relationship between pollutant production and process conditions. Process parameters include coal type, feeding technique, pressure, temperature and particle size, etc. (Concurrent to this report, two additional reports are being prepared, one dealing with identification of major process parameters and their influence on pollutant production, and the other dealing with vapor phase cracking and wet oxidation as potential pollutant control techniques for coal gasification.) Since the laboratory gasifier was used as a fixed-bed free-fall feed gasifier, the countercurrent flow of coal and gas gave rise to low bed exit temperatures resulting in high pollutant loadings. Thus the maximum pollutant concentrations (i.e., worst case) obtained from the gasifier are expected to be greater than, or at least near to, those obtained from large-scale gasifiers.

The objectives of this report dealing with a laboratory investigation of coal gasification are (1) to evaluate the relative environmental hazards associated with coal gasification effluent streams, (2) to evaluate the relative environmental hazards associated with individual constituents in each effluent stream, and (3) to compare the pollutant levels in the effluent streams with those from larger scale coal gasification and liquefaction units, combustion sources, ambient background levels, and regulated levels.

The reader should bear in mind that the effluent streams considered result from the gasification and quench steps and are not necessarily environmental discharges.

2.0 REACTOR, SAMPLING, AND ANALYSIS SYSTEMS

The RTI laboratory gasification reactor and measurement systems used in this study were described in previous reports.[1-4] Consequently, only a short description is presented here for the benefit of the reader. While different reactor configurations and processing conditions produce different effluent streams, a simple generalized flow sheet showing major inputs and outputs of a gasifier is given in Figure 1. What the authors wish to emphasize here is the difference between an entire gasification plant and the gasifier itself. Depending on the ultimate utilization pattern for the gas and the byproduct streams and the constraints on waste disposal, additional process equipment may be added. The laboratory gasification reactor has been fed primarily with coal, air, and steam to produce a low-Btu (150-200 Btu/scf) fuel gas in addition to the byproducts (i.e., tar, aqueous condensate, and ash). A variety of U.S. coals ranging from peat to anthracite have been gasified. Representative proximate and ultimate analyses of the fuels gasified are shown in Table 1.

2.1 REACTOR SYSTEM

A schematic diagram of the coal gasifier and sampling system is shown in Figure 2. The overall unit consists of a steam generation system, a gas feed system, a gasifier and nonvolatile sampling system, and a product gas sampling system. A PDP-11/34 data acquisition system with an Industrial Control Remote unit (ICR) is utilized to scan and store data on process conditions (i.e., temperatures, pressures, flows, condensate level, etc.). The gasifier has been constructed from a nominal 3-inch (7.6-cm), schedule 160, type 310 stainless steel, 46-inch (116-cm) long pipe. Above it is located a coal feed hopper and a coal feed system. The coal is fed under nitrogen pressure into the gasifier either in one batch of about 1.5 kg or continuously at 5-20 g/min. The batch feed system consists of a ball valve, whereas the continuous feed system enables coal to free-fall at a constant rate into the gasifier by means of a gear drive mechanism. The joints of the sight glass (which permits visual inspection of coal drop) are connected to the coal feed system with flanges at each end. The coal solids (generally 8 x 16 mesh in size) are supported about 15-inches from the bottom by means of a ceramic flow distributor plate. Air or nitrogen mixed with superheated steam enters the bottom of the reactor. The normal operating conditions for the reactor are 200 psig and 900°-1000°C at steam/coal and air/coal ratios to approximate large-scale low-Btu operations. Experimental conditions have been reported[3] in detail elsewhere on several gasification tests.

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EPA-287 (Cin.)
(4-76)

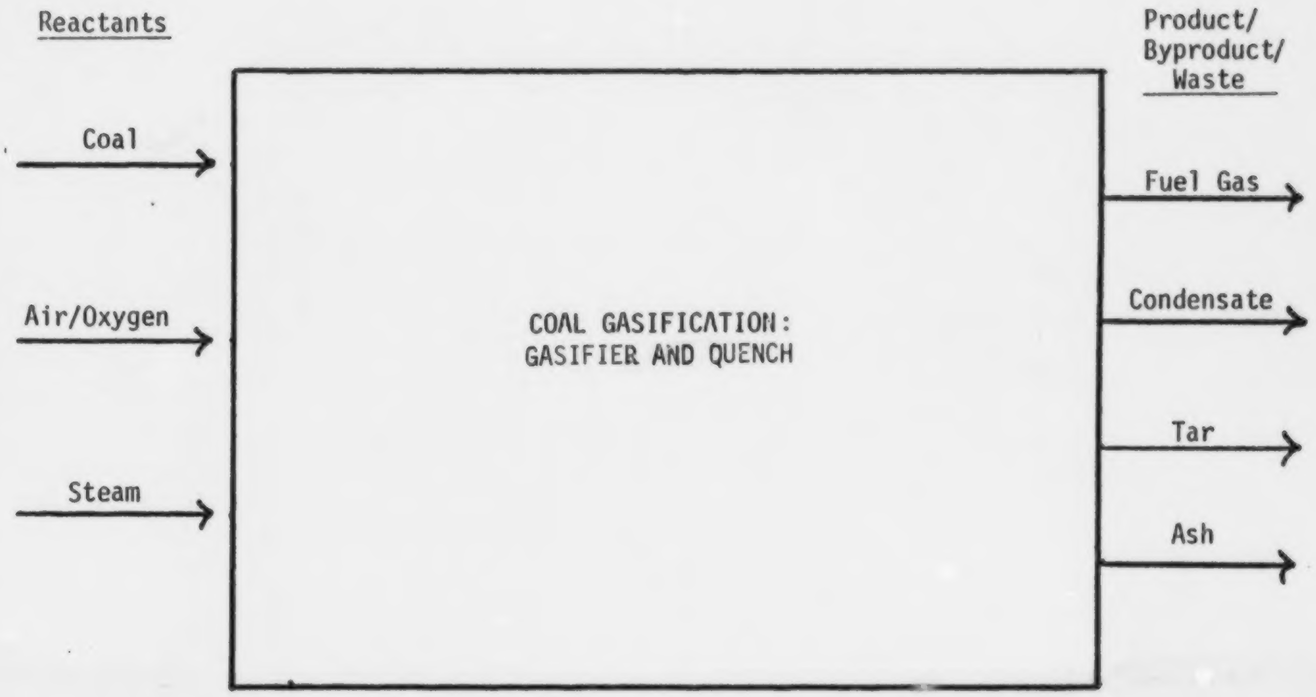
Reactants
Coal
Air/Oxygen
Steam
COAL GASIFICATION:
GASIFIER AND QUENCH
Product/
Byproduct/
Waste
Fuel Gas
Condensate
Tar
Ash

Figure 1. Coal gasification: influent and effluent streams.

TABLE 1. ANALYSIS OF FUELS GASIFIED AT RTI*

Fuel	Btu/lb	Moisture %	Ash %	Volatile Matter %	Fixed Carbon %	Sulfur %	Carbon %	Hydrogen %	Oxygen %	FSI	Ash Fusion Temp. °F	Nitrogen %
W. Kentucky FMC CHAR	11,090	1.00	19.70	7.80	71.50	1.80	74.02	1.48	1.70	< 1.0	2,600	1.3
Illinois No. 6 BITUMINOUS	11,331	6.85	13.52	32.58	47.05	3.01	63.26	5.37	13.46	3.5	2,280	1.38
Montana Rosebud SUB-BIT	9,004	21.19	8.86	31.56	38.39	0.59	53.96	6.87	28.53	0.0		1.20
N.C. Peat Humus	4,975	45.98	3.67	31.81	18.54	0.12	30.22	5.34	59.84	0.0		0.81
Pittsburgh No. 8	12,228	3.08	11.09	29.16	56.67	2.53	72.29	3.45	8.62	7		1.95
Wyoming SUB-BIT	8,225	15.56	6.31	38.30	39.83	0.55	56.80	5.94	30.02	0.0		0.38
N. Dakota Lignite	7,880	29.63	6.39	28.57	35.41	0.56	46.82	9.85	35.63			0.73
W. Kentucky No. 9 BITUMINOUS	12,130	7.03	7.83	38.78	46.36	4.44	67.69	5.55	13.30	4		1.08

*As received – %H and %O include that present in moisture.

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EPA-287 (Cin.)
(4-76)

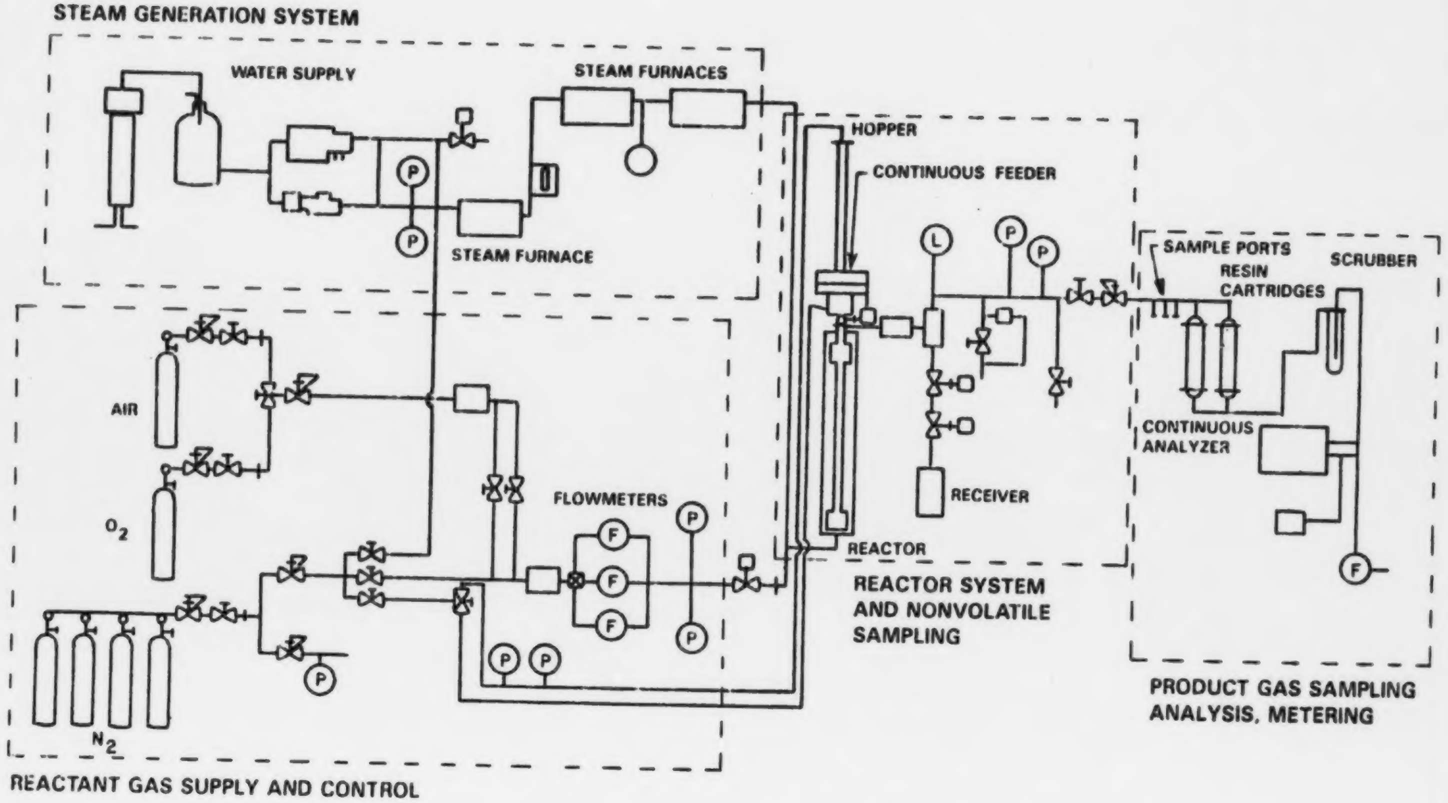
STEAM GENERATION SYSTEM
WATER SUPPLY
STEAM FURNACES
STEAM FURNACE
P
P
REACTANT GAS SUPPLY AND CONTROL
AIR
O_2
N_2
FLOWMETERS
F
F
F
P
P
P
P
P
HOPPER
CONTINUOUS FEEDER
REACTOR
L
P
P
RECEIVER
REACTOR SYSTEM AND NONVOLATILE SAMPLING
SAMPLE PORTS
RESIN CARTRIDGES
SCRUBBER
CONTINUOUS ANALYZER
F
PRODUCT GAS SAMPLING ANALYSIS, METERING

Figure 2. Laboratory gasifier and sampling system at RTI.

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(4-76)

2.2 SAMPLING SYSTEM

A detailed description of the sampling and analytical techniques are presented elsewhere.[2] Briefly, the sampling train can be broadly divided into a nonvolatile/semivolatile sampling system and a gas/vapor sampling system. The nonvolatile sampling system consists of a particulate trap and a condenser-receiver combination. The particulate trap (loosely packed with Pyrex wool) is a 12-inch (30-cm) section of 1-inch (2.5-cm) 316 stainless steel tube wrapped with a heater to maintain a temperature of 300°-500°C. The raw gas consisting primarily of N_2, H_2, CO, CO_2, CH_4, H_2O, and traces of tar, sulfur gases and volatile organics passes from the gasifier through the particulate trap to the jacketed condenser vessel with a holding capacity of up to 8 liters of aqueous condensate and tar. During a run the condensate is blown down periodically to a receiver vessel through a dual-valve pressure lock drain system. At the end of the run, the sample is acidified for preservation to a pH of ~ 2 and stored pending separation and analysis.

The noncondensibles consisting of gases and organic vapors pass through a backpressure regulator (thereby expanding to near ambient pressure) into a glass sampling system where a variety of samples including bulbs, glass fiber filter, sorbent resin (XAD-2^R), and impinger samples are collected. The glass sampling system is described in detail elsewhere.[2] Briefly, provision is made in the sampling approach to distinguish between the initial surge phase which occurs following the drop of the coal as a batch, and the pseudo steady-state which ensues when the rapid devolatilization and pyrolysis reactions are nearly complete. (Such a provision is not necessary during continuous feed gasification). Thus many gas bulb samples and one integrated filter/XAD-2 sample are collected during the surge phase. Relatively fewer gas bulb samples and an additional filter/XAD-2 sample are collected during the steady-state phase. In addition, the primary gases (H_2, CO, CO_2, and CH_4) are monitored continuously during the entire duration of the run by means of a thermal conductivity detector (for H_2) and three nondispersive infrared detectors (for CO, CO_2, and CH_4). Oxygen is also monitored using a paramagnetic analyzer primarily as a control measure (normally until run completion, no oxygen should be detected in the product gas) and to determine oxygen breakthrough (at run completion).

Overall, the samples collected during each gasification run include gaseous and liquid as well as solid samples. Schematically, the sample types are represented in Figure 3.

2.3 ANALYTICAL SYSTEM

As stated before, detailed description of most of the analytical techniques used is given elsewhere.[2] A brief description follows.

A schematic representation of the types of analyses performed and the instrumentation used are shown in Figure 4. This analytical scheme has continuously evolved through trial and error and experience gained from numerous samples during screening gasification runs. The solids (i.e.,

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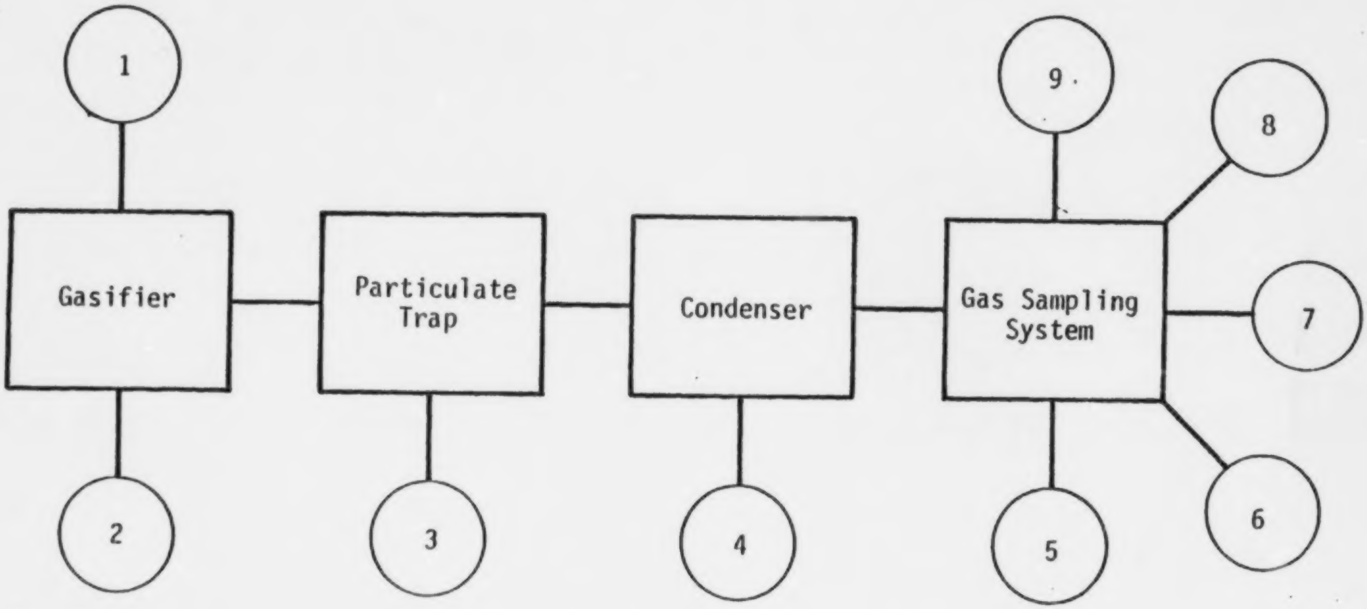
1
Gasifier
2
Particulate Trap
3
Condenser
4
9
Gas Sampling System
5
8
7
6

1. Coal
2. Residue
3. Particulates
4. Tar, Water and Insolubles
5. Entrained Tar and Water
6. Gas Bulbs
7. Polymeric Sorbents
8. Glass Fiber Filter
9. Scrubber Solutions

Figure 3. Samples collected during gasification of coal.

EPA-287 (Cin.)
(4-76)

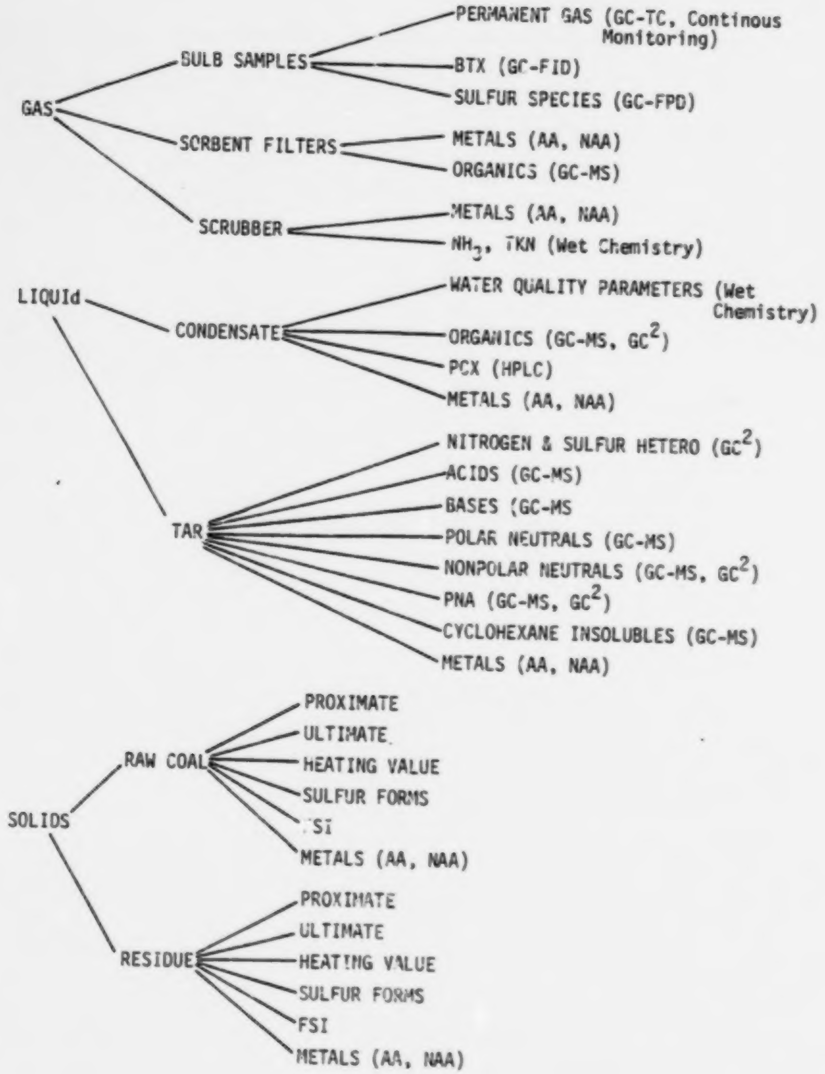
GAS
BULB SAMPLES
PERMANENT GAS (GC-TC, Continous Monitoring)
BTX (GC-FID)
SULFUR SPECIES (GC-FPD)
SORBENT FILTERS
METALS (AA, NAA)
ORGANICS (GC-MS)
SCRUBBER
METALS (AA, NAA)
NH$_3$, TKN (Wet Chemistry)
LIQUId
CONDENSATE
WATER QUALITY PARAMETERS (Wet Chemistry)
ORGANICS (GC-MS, GC^2)
PCX (HPLC)
METALS (AA, NAA)
TAR
NITROGEN & SULFUR HETERO (GC^2)
ACIDS (GC-MS)
BASES (GC-MS
POLAR NEUTRALS (GC-MS)
NONPOLAR NEUTRALS (GC-MS, GC^2)
PNA (GC-MS, GC^2)
CYCLOHEXANE INSOLUBLES (GC-MS)
METALS (AA, NAA)
SOLIDS
RAW COAL
PROXIMATE
ULTIMATE
HEATING VALUE
SULFUR FORMS
FSI
METALS (AA, NAA)
RESIDUE
PROXIMATE
ULTIMATE
HEATING VALUE
SULFUR FORMS
FSI
METALS (AA, NAA)

Figure 4. Analytical program.

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feed coal and reactor residue) are subjected to standard ASTM proximate and ultimate analyses as well as toxic trace elements analysis by atomic absorption (AA) and/or neutron activation (NAA). The gas samples can be divided into (1) gas bulb samples which are analyzed by standard gas chromatography[3] using a vacuum-pressure sample injection system, (2) XAD sorbents and filters which are exhaustively extracted by methylene chloride in a Soxhlet extractor, concentrated and analyzed by syringe injection onto a gas chromatography/mass spectrometry unit[2] for semivolatile to volatile organics such as naphthalene, phenol, pyridine, etc., and (3) acidic gas scrubber solutions which are analyzed for ammonia and total nitrogen (TKN) by classical wet chemistry and for trace metals by AA and/or NAA.

The liquid sample initially received from the gasifier condensate trap consists of a mixture of water and tar and is first separated by filtration. The aqueous portion is either exhaustively extracted by methylene chloride and analyzed as before by GC-MS or by direct aqueous injection with high pressure liquid chromatography (HPLC)/low wavelength ultraviolet (UV) detection (see Section 3.0 for details). The tar is analyzed directly by glass capillary gas chromatography (GC^2) for priority pollutants, nitrogen, and sulfur heterocyclics (see Section 3.0 for details). Also the tar is subjected to an elaborate solvent-partitioning scheme similar to the one employed by Novotny and coworkers[9] and described in detail elsewhere.[2,4] This separates it into six fractions which are acids, bases, polar neutrals, nonpolar neutrals, polynuclear aromatics, and cyclohexane insolubles. Each fraction is then qualitatively and/or quantitatively characterized by GC-MS or GC^2. Both tar and aqueous portions are analyzed by AA and/or NAA for trace metals. Data quality control for the entire sampling and analytical scheme is available elsewhere.[2]

2.4 PROBLEMS

Several problems have been encountered during the gasification program and methods have had to be intermittently updated as solutions have been found. However, a few problems still remain unresolved.

A major problem in reactor operations has been encountered during the gasification of high swelling index eastern coals, e.g., the Illinois No.6 coal or the Western Kentucky No.9 coal. During both batch feed as well as continuous feed, these coals have tended to agglomerate in the gasifier thereby resulting in poor gasification rates and heat transfer characteristics. To date, attempts to pretreat these coals (thereby reducing FSI) by a low temperature steam-air treatment, have not been successful, contrary to literature data.[10] One reason for this may be due to the rather large ratio of coal bed height to diameter in RTI tests. A possible approach that may be successful is continuous slow feed pretreatment of coal particles smaller than the 8 x 16 mesh particles used in this study. Pretreatment with catalysts such as K_2CO_3 and NaOH have been only marginally successful in reducing the caking properties. Continuous feed gasification has been carried out after mixing the coals with such moderators as limestone and wood pellets. A detailed description of the effect of these additives will be available in a companion report.

EPA-287 (Cin.)
(4-76)

Problem areas in sampling and analysis have been inadequate resolution of complex sample matrices, incomplete account of the nitrogen and sulfur compounds in the effluents, gaseous sulfur compound measurement in a complex organic matrix, breakthrough on polymeric sorbent materials, spillover of PNA compounds onto other tar fractions during solvent partitioning, and mass balance closures for trace elements. Major headways have recently been made by combining the resources of a GC-MS system to that of a GC^2 system with dual specific element detection (described in Section 3.0) for characterization of complex matrices. These techniques have also eliminated the need for elaborate tar fractionations. However, determination of high molecular weight sulfur heterocyclics and primary aromatic amines has not been possible primarily due to their presence at levels below detection limits of existing instrumentation. These compounds have recently been shown to be mutagenic[11,12] and it is important to determine their levels in coal gasification effluents.

Gaseous sulfur compounds which are measured by a flame photometric detector (FPD) are subject to response quenching when present in a complex organic matrix.[2,13] A dual flame FPD[14] minimizes this problem (and was utilized on this project) but does not eliminate it completely. When more accurate sulfur balances are required, attention needs to be given to alternate analysis techniques. Improper mass balance closures for trace elements are due to a combination of problems including analysis at ultra trace levels, and contribution or capture by the reactor and sampling systems themselves. Fortunately, only a few trace elements have been found to be present at environmentally significant levels in any of the effluent streams--arsenic being one of the predominant ones.

Another area of concern which was not properly addressed in this study is the formation of gaseous aerosols and fine particulates. Only brief attempts have been made to capture these using glass fiber filters upstream of the XAD resins. Analysis following extraction indicates the presence of up to five-ring compounds such as benzo(a)pyrene on the filters, thus warranting further investigation since if such compounds are confirmed to be present as suspended materials, estimated product gas toxicity could increase by many orders of magnitude.

Finally, another area that was not addressed in a systematic manner in this study is that of fugitive emissions which are known to be a problem in the operation of chemical process plants. However, these emissions are dependent on a multitude of factors related to individual processes. A sufficient data base on the effluent streams from coal gasification has been compiled which may be of use in predicting fugitive emissions from integrated coal gasification facilities.

3.0 SPECIAL ANALYTICAL TECHNIQUES

A brief description of the analytical techniques which were used was given in Section 2.3. Two techniques which were recently developed and successfully applied deserve special mention. These are described below.

3.1 PCX IN CONDENSATE BY HPLC/LOW WAVELENGTH UV

Although traditionally such techniques as the 4-aminoantipyrine method[15] and gas chromatography[16] are used to measure phenol, cresols, and xylenols (PCX) in water, these methods are either lengthy or indirect involving solvent extraction. Difficulty in solvent extracting phenols from water is well known[17] and this is what prompted the development of the high pressure liquid chromatography (HPLC) technique described below. Although reverse phase HPLC analysis of phenolics is straightforward, group quantitation of three isomeric cresols and six isomeric xylenols is more challenging. The method development required the use of low efficiency columns [N=1000] (which also resulted in increased longevity and reduced cost) to elute phenol as one peak, all cresols as one peak, and all xylenols as one peak. Low wavelength UV (215 nm) was required so that absorbance of all cresols became similar and of all xylenols became similar. Thus, calibration curves could be prepared with only one cresol and one xylenol with 4-isopropylphenol as the internal standard. As expected, for aqueous condensate from the gasifier, direct aqueous injection became feasible with phenol eluting first followed by cresols (one peak) and xylenols (one peak). The method was simpler, more cost-effective, and more accurate compared to the GC method and has been routinely applied in coal gasifier condensate samples. A more detailed description is available in a recent publication by Sparacino and Minnick.[18]

3.2 GLASS CAPILLARY GAS CHROMATOGRAPHY (GC^2)

The difficulty encountered in characterizing complex mixtures such as tar and aqueous condensate organics by GC-MS in a cost-effective manner, motivated the development of a direct GC^2 technique. This technique has been reported in detail in two papers[19,20] and only a brief description will be presented here.

It became quite clear upon analyzing the cyclohexane insoluble and the polar neutral tar fractions that certain amounts of PNAs were spilling over to these fractions. Thus, a technique which could analyze tar without prior fractionation was needed. In addition, from GC-MS results it was also clear that this expensive device was excellent for identification purposes but was not quite sensitive enough to quantitate ultra trace amounts of sulfur and nitrogen compounds. Therefore, sensitive techniques complementary to GC-MS were needed.

Analysis methods were developed using two GC^2 systems, one consisting of a flame ionization detector (FID) and a dual-flame photometric detector (FPD) for simultaneous analysis of PNAs and sulfur compounds and the other consisting of a FID and a nitrogen-phosphorus detector (NPD) for simultaneous analysis of PNAs and nitrogen compounds. Each system was equipped with a wall coated 25 m x 0.25 mm OV-101 capillary column. Sample injection was performed using the "splitless technique" of Grob and Grob.[21] Preliminary qualitative sample analysis by GC-MS was followed by a more rigorous quantitative analysis using an internal standard with the GC^2 systems. Typical analytical chromatograms for crude tar samples from recent runs are shown in Figures 5, 6, and 7 for the FID, FPD, and NPD, respectively. The large number of compounds identified and quantitated[20] demonstrates the utility of the technique. The technique is flexible because it affords a larger sample size than the GC-MS technique and thus has a lower detection limit. In addition, identification is facilitated by the use of specific and highly sensitive detectors.

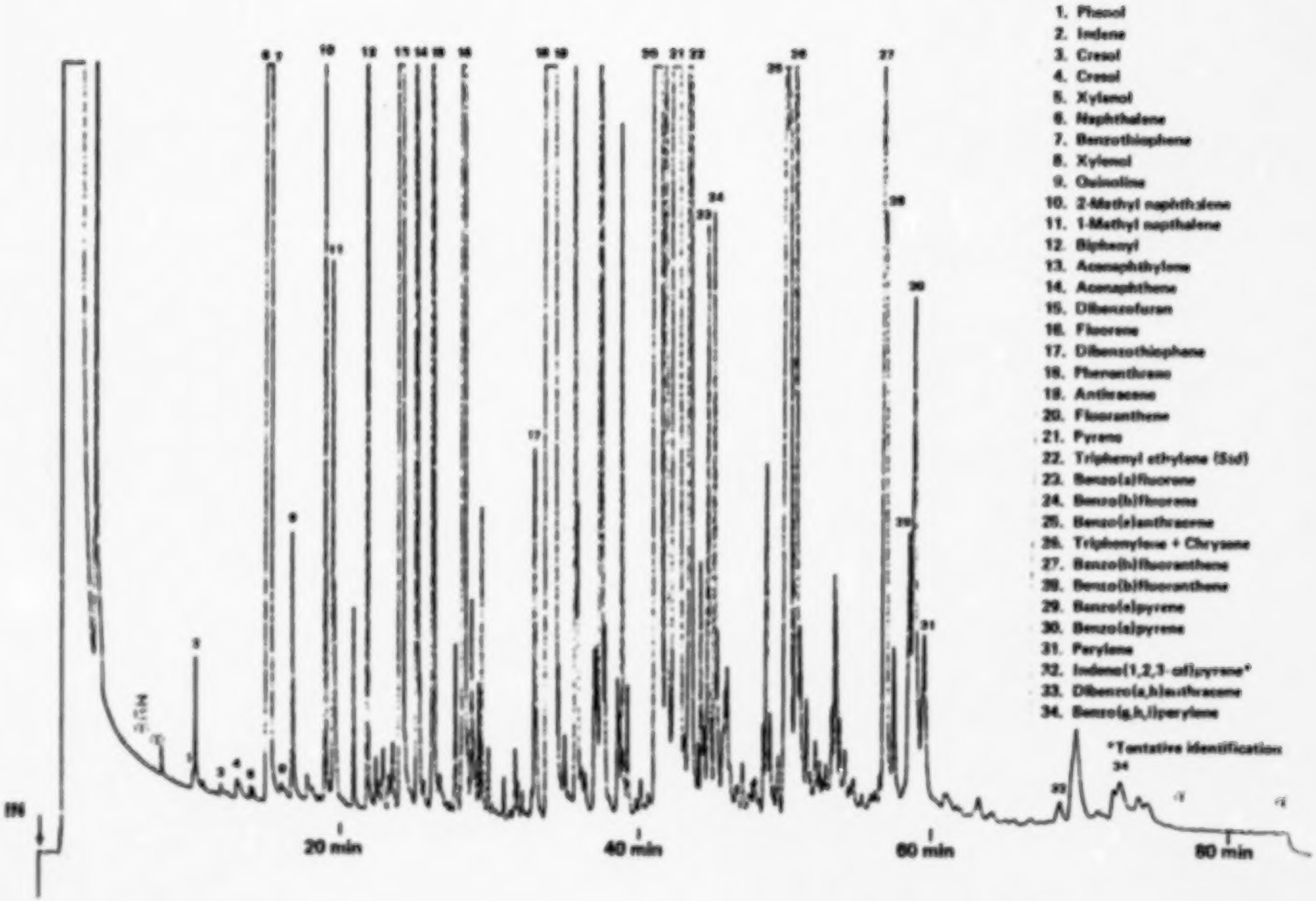

Figure 5. FID chromatogram of crude tar from gasification of Wyoming coal (Run C2).

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EPA-287 (Cin)
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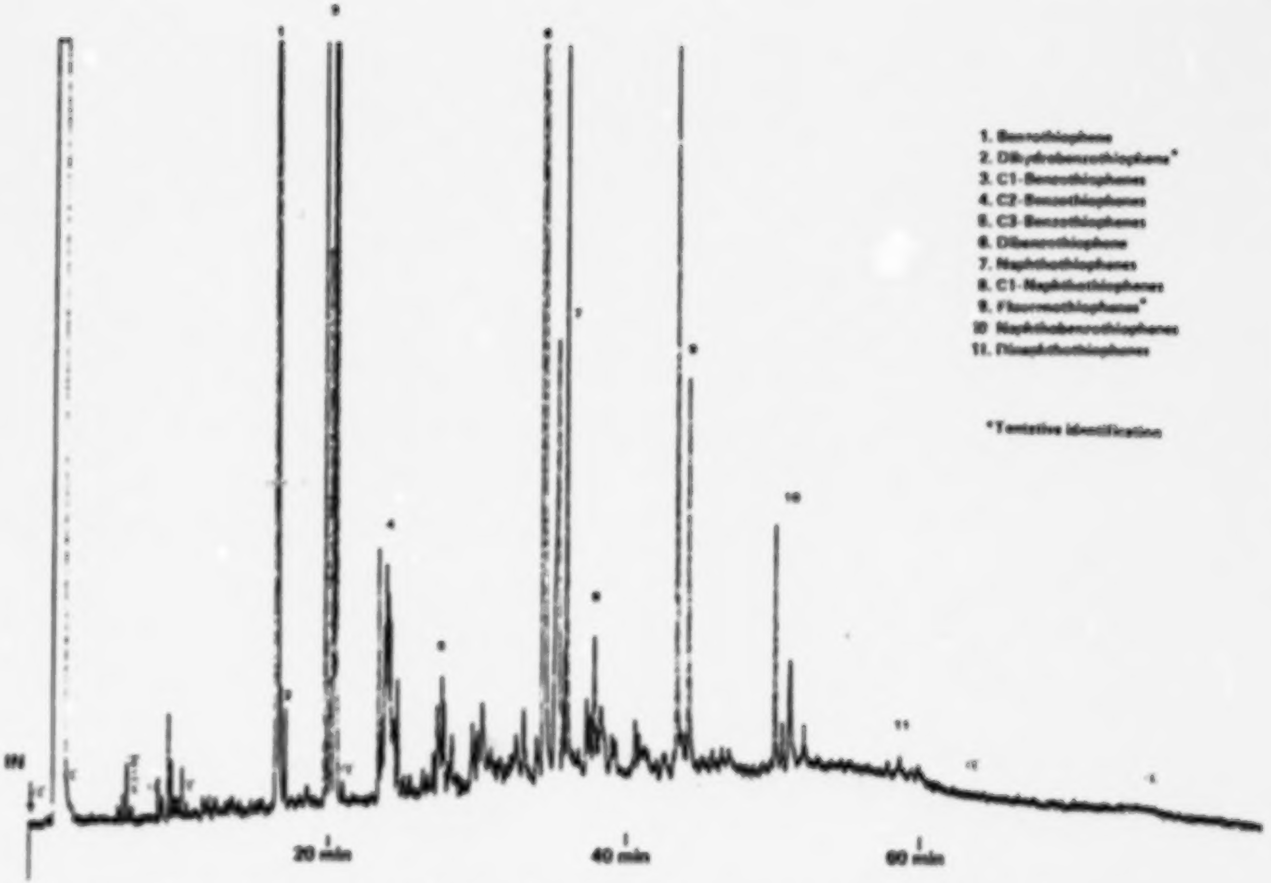

Figure 6. FPD chromatogram of crude tar from gasification of a mixture of Illinois No.6 coal and limestone (Run C6).

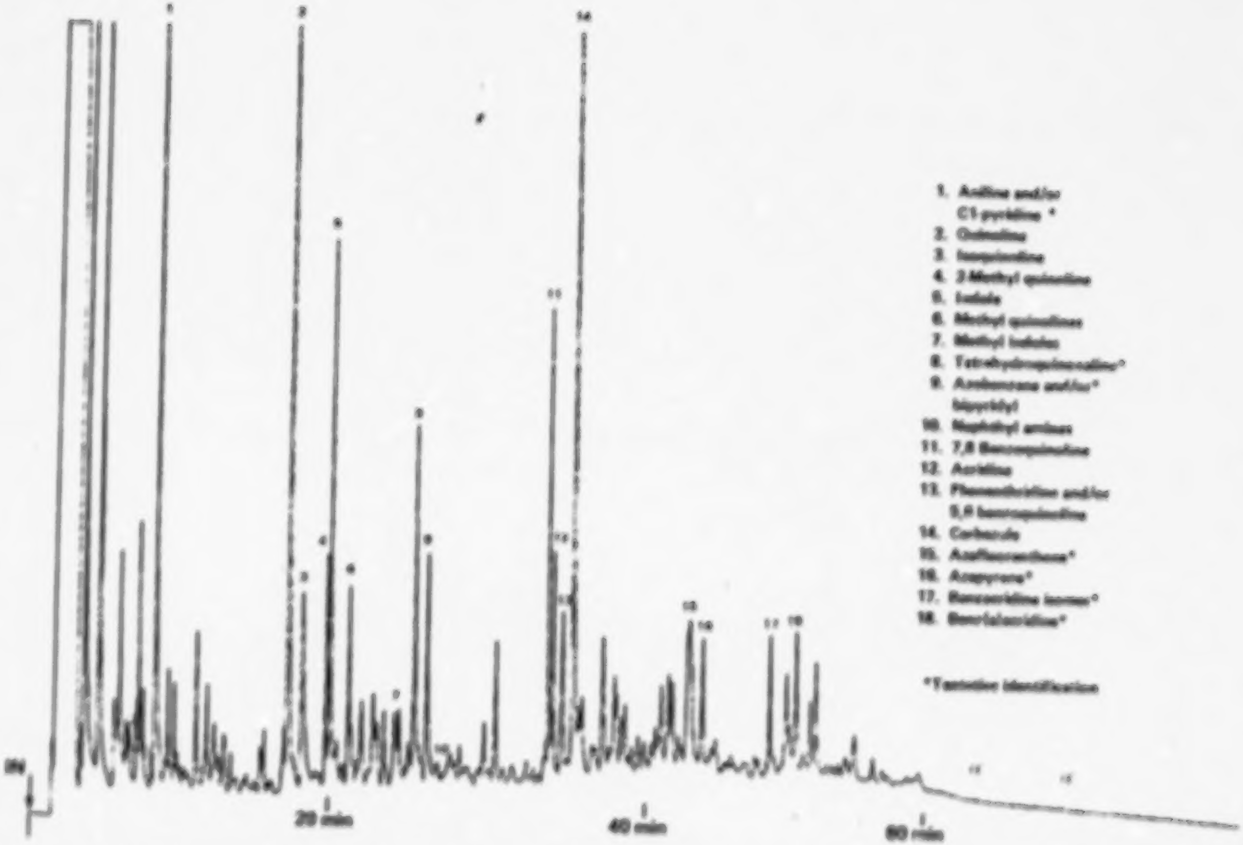

Figure 7. NPD chromatogram of tar from gasification of a mixture of Illinois No.6 coal and $CaCO_3$ (Run C6).

4.0 MEG METHODOLOGY AND BIOASSAY

The need for an environmental assessment methodology was given impetus by the increased importance of energy independence for the United States. The EPA began the systematic development of a method with several components for environmental assessment about five years ago. Two of these components are "multimedia environmental goals" (MEGs) and biological testing of samples (bioassay). These two, especially for complex samples such as those derived from synfuels processes, complement each other quite well in assessing the environmental hazard associated with pollutants. Since detailed reports have been compiled on each (references 5-8 for MEGs, references 22-24 for bioassay) only a brief description of the procedures is presented here as they relate to those used in this report.

4.1 MEG METHODOLOGY

MEG methodology (although not a standard or regulation) provides a means to quantitate the control of pollutants necessary in emissions to the environment (land, water or air) from process operations. On the basis of available toxicity and biological data, the methodology provides concentrations (discharge multimedia environmental goal, DMEG) for more than 600 chemical species. A DMEG is a concentration of a pollutant is an undiluted effluent stream which will not adversely affect people or ecological systems exposed for short periods of time. DMEG is further classified into a health DMEG ($DMEG_H$) or an ecological DMEG ($DMEG_E$). Only $DMEG_H$ values are used in this report for environmental assessment of coal gasification effluent streams. The units used for DMEGs are $\mu g/m^3$ for product gas, $\mu g/L$ for aqueous condensate, and $\mu g/g$ for tar and ash.

A word of caution is needed here in regard to the use of DMEGs. First, they are not to be regarded as regulations. They are only designed to rank chemicals in an effluent stream on the basis of predicted environmental acceptability. Both DMEGs and models from which they are derived are bsed frequently on limited data whose reliability has not been confirmed. Also the methodology is continuously evolving as new data become available for chemicals which have already been assigned DMEGs or for new chemicals.

In the assessment methodology used in this report, quantitative analysis of an effluent stream's constituents is first performed. Then discharge severity (DS) for each of these constituents is determined as follows:

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EPA-287 (Cin.) (6-06)

$$DS_i = \frac{C_i}{DMEG_i} \qquad (1)$$

where DS_i = discharge severity of the ith constituent.

C_i = concentration of the ith constituent.

$DMEG_i$ = health DMEG for the ith constituent.

A DS value of one or less for a constituent in a stream implies that the constituent is present at environmentally insignificant levels. The constituents are ranked in the order of the discharge severity. The most important constituents are thus obtained from an environmental (health) standpoint. Also constituents whose DS values are consistently below unity can be eliminated as potential hazards. An overall discharge severity of effluent streams can also be determined by summation of the discharge severities of their constituents. Further details on the use of the MEG methodology is available in Section 5.0 where results are presented about the various compounds in the effluents from the laboratory coal gasifier.

4.2 BIOASSAY

The Level 1 environmental assessment approach for screening environmentally significant samples includes a series of short-term bioassays for the detection of acute biological effects.[22] This includes both health-related and ecological tests. The health tests are provided to screen for both acute toxic and potential chronic (i.e., carcinogenic) health effects. The tests include the Ames Salmonella typhimurium reverse mutation assay, the Chinese hamster ovary (CHO) cells, cytotoxicity assay, the rabbit alveolar macrophage (RAM), aquatic ecological tests, and other suggested procedures. Only the first two were employed in this study, and a short description of each follows. Details of the actual laboratory procedures are available in an earlier report.[4]

4.2.1 Ames/Salmonella Reverse Mutation Bioassay

The bacterial mutagenesis bioassay is the most highly developed and validated test for chemical mutagens used currently in biotesting programs. The assay employs five Salmonella strains mutated at the histidine locus, rendering them unable to grow in agar medium deficient in histidine. Two of the strains have increased sensitivity to chemical mutagens because they possess a DNA plasmid with an extra copy of the mutated histidine locus. When the histidine mutation is reverted by the action of a chemical mutagen, the bacteria are able to form visible colonies on histidine-deficient agar. Colony formation has been demonstrated to be quantitatively related to the potency and dose of chemical mutagen administered. This assay has been so widely used as an indicator of mutagenic potential that standardized protocols have been developed for its use, and extensive validation studies have demonstrated a rather good correlation between the mutagenic and carcinogenic potencies of many chemical substances. The Ames assay has also been demonstrated to be an effective indicator of the mutagenicity of complex environmental organic mixtures.

Disadvantages of the Ames assay are that it detects only reverse mutations, there have been a number of false negative and false positive responses noted for this system; it will not detect promutagens/procarcinogens in the absence of an externally supplied metabolic activation system, and it is a prokaryotic system physiologically different from mammalian systems.

4.2.2 Chinese Hamster Ovary (CHO) Cell Cytotoxicity Assay

Mammalian cells, such as the Chinese Hamster Ovary (CHO) cell, grown in tissue culture serve as a substitute for the whole animal as a screening tool for assessing the cellular toxicity of xenobiotics to mammals. The putative toxins challenge the cells by addition to the growth medium when the cells are growing as a monolayer, attached to a plastic substrate. Inhibition of cell growth is determined either in the growth kinetics mode or the cloning efficiency mode. In the former some 100,000 cells are exposed to the compound of interest and the growth curve evaluated whereas in the latter, only a few (100-500) cells are exposed to determine the ability of single cells to produce viable colony of cells. The CHO cells are especially suited for these cytotoxicity assays because they possess a constant chromosome number, are fairly resistant to infections, are relatively easy to maintain in a culture, and divide rather rapidly (12-14 hours doubling-time), and exhibit consistent growth when cultured under standard conditions.

5.0 RESULTS

As discussed in Section 2.0, four distinct streams emerge from the laboratory coal gasifier. These are designated as product gas, tar, aqueous condensate, and ash. Each stream is then analyzed for their constituents. To date, more than 400 compounds have been identified in the various effluent streams. In addition, some 100 compounds were quantitated in more than 30 gasification tests. An attempt is made in this section to present these quantitative results (which represent a massive amount of information) in a meaningful manner so that the relative environmental (health) hazards for each stream and their constituents can be determined.

5.1 STREAM CONCENTRATIONS

The concentration of the pollutants in the various streams are expressed as μg/m^3 for gas, μg/L for aqueous condensate, and μg/g for ash and tar in order to retain consistency with DMEGs which are also expressed in these units. The concentrations are an average integrated concentration for the entire duration of the test. Thus total ash, tar, and water are collected at the end of the test, and representative aliquots of each are analyzed to determine the concentrations. For the product gas, bulbs are collected as grab samples at various times during a test. Since the flow rate of the gas is recorded, it is straightforward to obtain an integrated concentration for the gas as well.

No attempt has been made in this report, as stated in Section 1.0, to correlate operating conditions during a test to pollutant production (this information will be available in a companion report). Rather, the entire range of concentrations obtained over all tests for all significant pollutants are presented. Only in a few instances, such as for bioassay results (Section 5.4), is the effect of coal type shown.

5.1.1 Significant and Nonsignificant Constituents

Determination of the significance or nonsignificance of a pollutant in a stream is made by comparing the maximum concentration observed among all tests to the corresponding health DMEG value. Tables 2 through 5 show the constituents in the four streams which are eliminated from consideration. All these constituents have an assigned DMEG based on MEG models. However, some of the constituents which were present at very low concentrations but did not have an assigned DMEG could not be completely eliminated from consideration. These and others whose maximum concentration exceeded the DMEG are shown in Tables 6 through 9. An assignment of DMEG was made to various constituents (which do not have one) in these tables on the basis of

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EPA-287 (Cin.)
(4-76)

TABLE 2. PRODUCT GAS CONSTITUENTS ELIMINATED BASED ON MAXIMUM CONCENTRATION

ethane and higher alkanes (also substituted)
ethylene and higher alkenes (also substituted)
acetylene and higher alkynes (also substituted)
ethylbenzene
benzaldehyde
styrene
indan
methylnaphthalenes
anthracene
pyrene
fluoranthene
aniline
pyridines
quinolines
C_3-thiophenes
C_4-thiophenes
benzothiophenes

EPA-287 (Cin.)
(4-76)

TABLE 3. AQUEOUS CONDENSATE CONSTITUENTS ELIMINATED BASED ON MAXIMUM CONCENTRATION

naphthalene
methyl naphthalenes
anthracene
phenanthrene
chrysene
fluoranthene
benzo(e)pyrene
benzo(k)fluoranthene
benzo(b)fluoranthene

Elements

phosphorus
aluminum
antimony
beryllium
cobalt
copper
manganese
mercury
scandium
sodium
zinc

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TABLE 4. TAR CONSTITUENTS ELIMINATED BASED ON MAXIMUM CONCENTRATION

	Trace elements
aniline	antimony
benzidine	cadmium
C_2-alkylnaphthalenes	cobalt
1-methyl naphthalenes	copper
2-methyl naphthalenes	iron
anthracene	lead
methyl anthracenes	manganese
fluorene	mercury
fluoranthene	nickel
benzo(e)pyrene	scandium
benzo(k)fluoranthene	selenium
benzo(b)fluoranthene	sodium
indeno(1,2,3-cd)pyrene	zinc
quinoline	beryllium
acridine	
indole	
carbazole	
isoquinoline	
2-methyl quinoline	
methyl indoles	
1-amino naphthalenes (6 observations only)	
2-amino naphthalenes (6 observations only)	
7,8-benzoquinoline	
phenanthridine	
phenyl pyridine	
aza pyrene	
benzoacridines	
benzothiophene	

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TABLE 5. ASH ELEMENTS ELIMINATED BASED ON MAXIMUM CONCENTRATION

antimony
cadmium
cerium
cobalt
copper
lanthanum
lead
magnesium
mercury
rubidium
samarium
thorium
titanium
uranium
vanadium

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EPA-287 (Cin.)
(4-76)

TABLE 6. PRODUCT GAS CONSTITUENTS NOT ELIMINATED BASED ON MAXIMUM CONCENTRATION

Exceed $\text{DMEG}_{\text{health}}$	No $\text{DMEG}_{\text{health}}$
methane	hydrogen*
methanethiol	C_3-benzenes$^+$
ethanethiol	C_4-benzenes$^+$
benzene	diphenylmethane*
toluene	acenaphthene*
xylenes	fluorene$^+$
thiophene	benzofuran$^+$
methylthiophenes	methylbenzofuran$^+$
dimethylthiophenes	dibenzofuran$^+$
carbon monoxide	
carbon dioxide	
ammonia	
hydrogen cyanide	
hydrogen sulfide	
carbonyl sulfide	
carbon disulfide	
biphenyl	
indene	
phenanthrene	
phenol	
cresols	
xylenols	
naphthalene	

*Exceeds DMEG conservatively assigned based on lowest DMEG in category. Need further study to determine hazard potential and DMEG.

$^+$Do not exceed assigned DMEG.

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PAGE NUMBER
EPA-287 (Cin.)
(4-76)

TABLE 7. AQUEOUS CONDENSATE CONSTITUENTS NOT ELIMINATED BASED ON MAXIMUM CONCENTRATION

Exceed DMEG$_{health}$	No DMEG$_{health}$
phenol	acenaphthylene[+]
cresols	triphenylene[+]
xylenol	fluorene[+]
trimethylphenols	perylene[+]
benzo(a)pyrene	nitrates[+]
cyanide	thiocyanates*
ammonia	
chlorides	
sulfides	
Trace Elements	
arsenic	
cadmium	
chromium	
iron	
lead	
selenium	
silver	

*Exceeds DMEG conservatively assigned based on DMEG for cyanide. Need to develop a proper DMEG based on further experiments.

[+] Do not exceed DMEG assigned based on lowest DMEG in category.

TABLE 8. TAR CONSTITUENTS NOT ELIMINATED BASED ON MAXIMUM CONCENTRATION

Exceed DMEG$_{health}$	No DMEG$_{health}$
biphenyl	acenaphthene*
phenol	acenaphthylene*
cresols	triphenylene*
xylenols	perylene*
trimethylphenol	benzo(g,h,i)perylene*
naphthalene	benzo(a)fluorene$^+$
phenanthrene	benzo(b)flurorene$^+$
benzo(a)anthracene	dibenzothiophene$^+$
chrysene	methyl benzothiophenes$^+$
pyrene	C_2-benzothiophenes$^+$
dibenzo(a,h)anthracene	C_3-benzothiophenes$^+$
benzo(a)pyrene	naphthothiophenes**
	phenanthro(4,5-bcd) thiophene**
	napthobenzothiophenes**
	dinaphthothiophenes**
Trace elements:	
arsenic	
chromium***	

---

*Exceed DMEG conservatively assigned based on lowest DMEG in category. Need further biological and toxicity studies.

$^+$Do not exceed assigned DMEG based on lowest DMEG in category.

**Not enough information to assign DMEG. Need further biological and toxicity studies.

TABLE 9. ASH ELEMENTS NOT ELIMINATED BASED ON MAXIMUM CONCENTRATION

Exceed $\text{DMEG}_{\text{health}}$	No $\text{DMEG}_{\text{health}}$
aluminum	chlorine[+]
arsenic	bromine[+]
beryllium	
chromium	
iron	
manganese	
nickel	
selenium	
sodium	

[+] Do not exceed DMEG assigned based on lowest DMEG in category.

the lowest DMEG in the MEG category.[5-8] This is actually the most conservative assignment that can be made on the basis of present knowledge. Even after such a conservative assignment, many more constituents in each stream were eliminated. These are shown in the right hand columns of Tables 6 through 9 with a "+" superscript. Several other constituents in the right-hand columns with a superscript "*" exceed the assigned DMEG and so do all the constituents in the left-hand columns (these already have DMEGs).

It appears that the biggest information gap for DMEGs exists for the tar stream constituents, because it was not possible to even assign a DMEG for sulfur heterocyclics that were identified. Recently, as stated in Section 2.0, some of these compounds (notably phenanthro(4,5-bcd)thiophene) have been shown to exhibit mutagenic activity.[11] A definite need exists to develop a proper DMEG for these compounds. It is to be noted from Table 3, that the aromatic amines that are generally considered to impart mutagenic activity to coal liquefaction samples[12] were actually eliminated from consideration from the coal gasification tar samples on the basis of six observations. This is further discussed in conjunction with the bioassay results in Section 5.4.

Another point of interest is the presence of chromium as a significant constituent in the tar, aqueous condensate, and ash streams. The ash stream further had nickel and manganese as significant constituents. It is believed that these are caused primarily due to an artifact of the stainless steel reactor which at high gasification temperatures contributes these elements to the various streams.

5.1.2 Discharge Severity

After eliminating the nonsignificant constituents, the next step was to rank the significant constituents on the basis of their discharge severity in the various streams, i.e., to determine their relative hazard potentials. Here discharge severity is defined as the mean concentration divided by the DMEG (see Equation (1)). The ranks and the discharge severities of the various constituents in the four streams are shown in Tables 10 through 13. For product gas in Table 10, it is to be noted that the products that one is trying to make (i.e., carbon monoxide and hydrogen) are among the top five as far as the relative hazards of the constituents are concerned. Further eliminations of constituents from consideration are possible based on Tables 10 through 13. If one assumes mean concentrations and not maximum concentration as the bases for elimination, then one can further eliminate the constituents receiving discharge severities less than or close to unity. If DS $\geq$ 10 is considered the cutoff point instead of DS $\geq$ 1, then only fixed gases, benzene, and sulfur species remain significant for product gas. Ash becomes almost nonhazardous because arsenic and chromium are the only elements with a discharge severity above 10. Chromium, in addition, is believed to be an artifact of the stainless steel reactor. In tar only cresols, xylenols, and higher polynuclear aromatic hydrocarbons need to be considered. Aqueous condensate is the only stream in which more than 10 constituents exceed a discharge severity of 10. It is to be noted that cresols and xylenols dominate in rank for both aqueous condensate as well as

EPA-287 (Cin.) (4-76)

TABLE 10. PRODUCT GAS CONSTITUENTS RANKED ON THE BASIS OF DISCHARGE SEVERITY: (Mean Concentration/DMEG)

	Rank	Discharge Severity
carbon monoxide	1	5800
benzene	2	700
hydrogen sulfide	3	300
carbonyl sulfide	4	55
hydrogen*	5	37
carbon dioxide	6	28
thiophene	7	18
methanethiol	8	14
ethanethiol	9	8.4
methane	10	7.9
xylenols	11	7.0
carbon disulfide	12	6.3
cresols	13	6.2
phenol	14	5.8
ammonia	15	5.0
hydrogen cyanide	16	4.4
biphenyl	17	2.9
methyl thiophenes	18	2.8
naphthalene	19	2.4
indene	20	1.8
toluene	21	1.4
acenaphthene*	22	1.3
dimethyl thiophenes	23	1.2
diphenyl methane*	24	0.9
phenanthrene	25	0.5
xylenes	26	0.4

*No DMEG exists. Rank is based on lowest DMEG in category.

TABLE 11. AQUEOUS CONDENSATE CONSTITUENTS RANKED ON THE BASIS OF DISCHARGE SEVERITY: (Mean Concentration/DMEG)

	Rank	Discharge Severity
cresols	1	120,000
xylenols	2	50,000
trimethyl phenol	3	3,600
ammonia	4	2,600
sulfides	5	880
arsenic	6	330
thiocyanates*	7	230
benzo(a)pyrene	8	120
phenol	9	71
cadmium	10	18
selenium	11	13
chromium[+]	12	7
cyanide	13	4.4
iron	14	3.3
chlorides	15	2.6
silver	16	1.1
lead	17	0.6

*DMEG assigned equal to that for cyanide.

[+] These may be significantly contributed by the stainless steel reactor.

TABLE 12. TAR CONSTITUENTS RANKED ON THE BASIS OF DISCHARGE SEVERITY: (Mean Concentration/DMEG)

	Rank	Discharge Severity
cresols	1	17,000
xylenols	2	12,000
trimethylphenol	3	3,100
dibenzo(a,h)anthracene	4	500
benzo(a)pyrene	5	420
perylene*	6	300
triphenylene*	7	270
benzo(a)anthracene	8	31
benzo(g,h,i)perylene*	9	7.7
phenanthrene	10	6.3
arsenic	11	5.3
naphthalene	12	4.7
acenaphthylene*	13	4.6
pyrene	14	2.4
phenol	15	2.3
biphenyl	16	1.1
acenaphthene*	17	0.9
chromium+	18	0.7
chrysene	19	0.6

+This is very likely due to the stainless steel reactor which contains substantial amounts of chromium.

*No DMEG exists. Rank is based on lowest DMEG in category. Need further biological and toxicity data to determine DMEG.

TABLE 13. ASH ELEMENTS RANKED ON THE BASIS OF DISCHARGE SEVERITY: (Mean Concentration/DMEG)

	Rank	Discharge Severity
arsenic	1	45
chromium*	2	32
nickel*	3	7.2
manganese*	4	5.4
iron	5	4.8
beryllium	6	4.3
aluminum	7	4.0
sodium	8	1.9
selenium	9	0.4

*This is likely due to the contribution of the stainless steel reactor.

tar. For aqueous condensate, they are expected to dominate because of their low DMEGs and high water solubility. The dominance of cresols and xylenols in tar and aqueous condensate is discussed in conjunction with overall stream hazard evaluations in Section 5.3.

5.1.3 Concentration Ranges

The ranges of concentrations of significant pollutants in all gasification tests for the various streams are shown in Figures 8 through 12. Figures 8 and 9 correspond to the product gas constituents, the former showing the most significant constituents and the latter showing constituents of medium significance. Figures 10, 11, and 12 are for constituents in the aqueous condensate, tar, and ash streams, respectively.

The figures are plots of the concentrations versus the DMEG. Thus the 45° line corresponds to concentration = DMEG. The concentration bars include the minimum, maximum, arithmetic mean, geometric mean, and 95 percent confidence interval for each pollutant in each stream. The significance of the 45° line is that it allows easy visual inspection of the relative degree of significance and relative hazard of the various constituents. The higher the bars or means are above the 45° line, the higher the hazards. Also constituents plotted on the left of the figures have lower DMEGs and are consequently more hazardous at the same concentration levels.

5.2 PRODUCTION FACTORS AND CONTROL PRIORITIES

From the concentration of the pollutants in the various streams, their DMEGs and the amount of coal gasified, two useful quantities can be determined for each pollutant in each stream. These are the production factors (PF) and the control priorities (CS). These quantities are defined, determined, and graphed in the following subsections.

5.2.1 Production Factors

Production factor is defined here as the ratio of the weight of a pollutant in an effluent stream to the weight of coal gasified.

$$\text{Production Factor} = \frac{\text{weight of pollutant}}{\text{weight of coal gasified}} \qquad (2)$$

For convenience the unit chosen for production factor is μg/g. Figures 13, 14, 15, and 16 present production factors of significant pollutants in gas, aqueous condensate, tar, and ash, respectively. The pollutants in these figures are listed in the order of increasing discharge severity from left to right. The figures present the ranges of production factors found in all tests including minimum, maximum, arithmetic mean, geometric mean, and 95 percent confidence interval. The usefulness of these figures becomes clear when one considers that it gives an immediate account of how much of a constituent to expect from the coal gasifier, i.e., how much of a byproduct can be produced (e.g., ammonia and phenol from the aqueous condensate) or how much of a pollutant needs to be controlled (e.g.,

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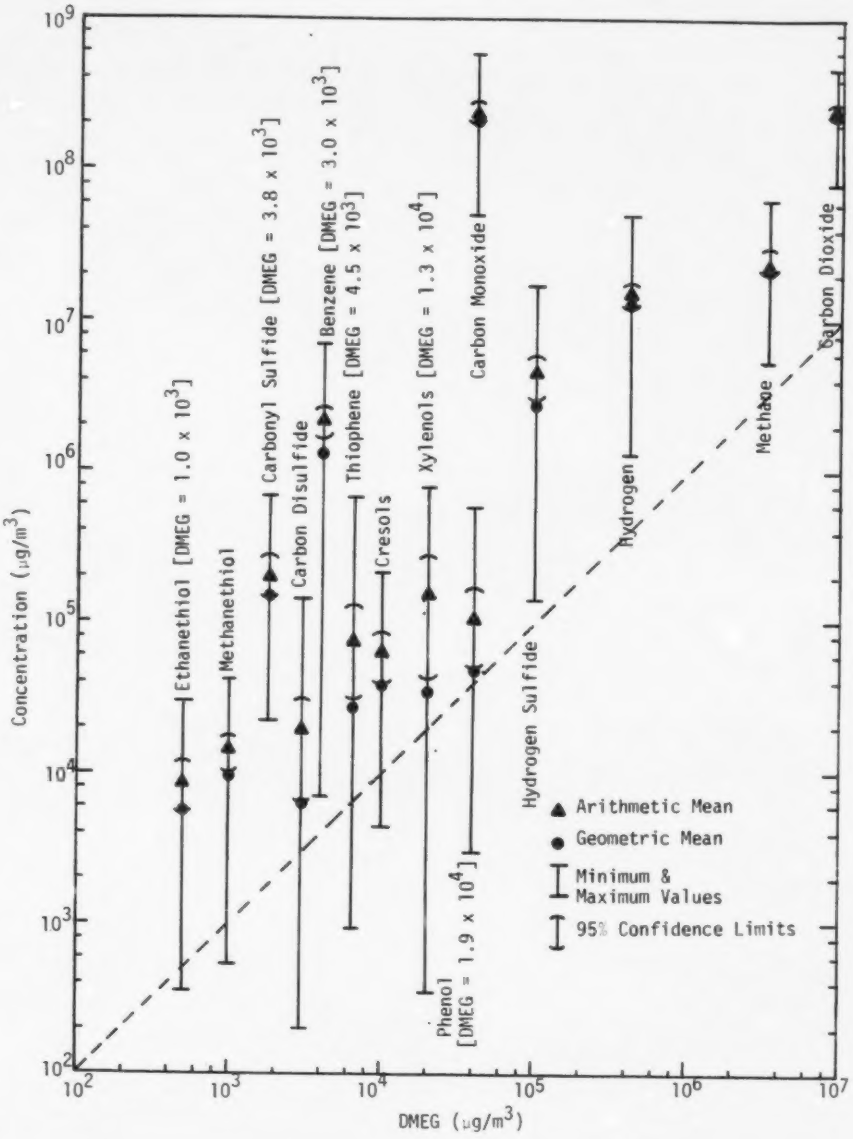

Figure 8. Ranges of concentrations for most significant product gas constituents.

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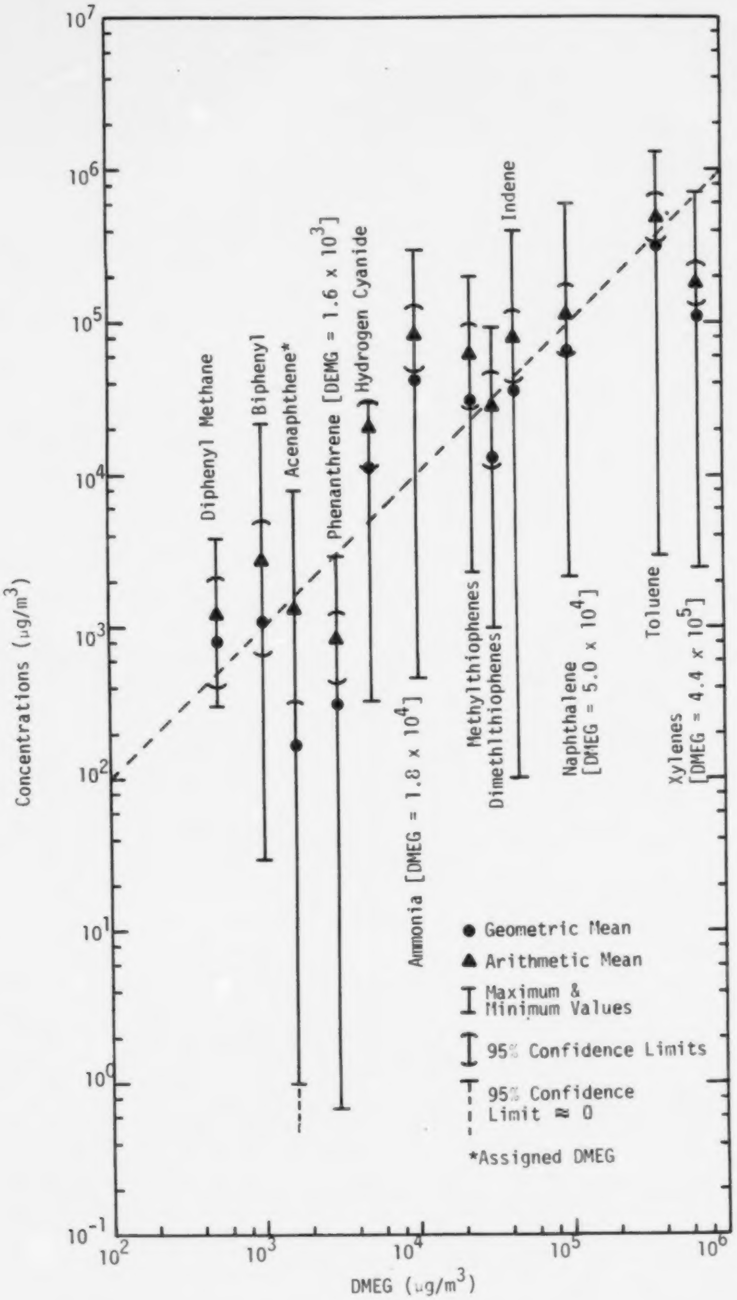

Figure 9. Ranges of concentrations for product gas constituents of medium significance.

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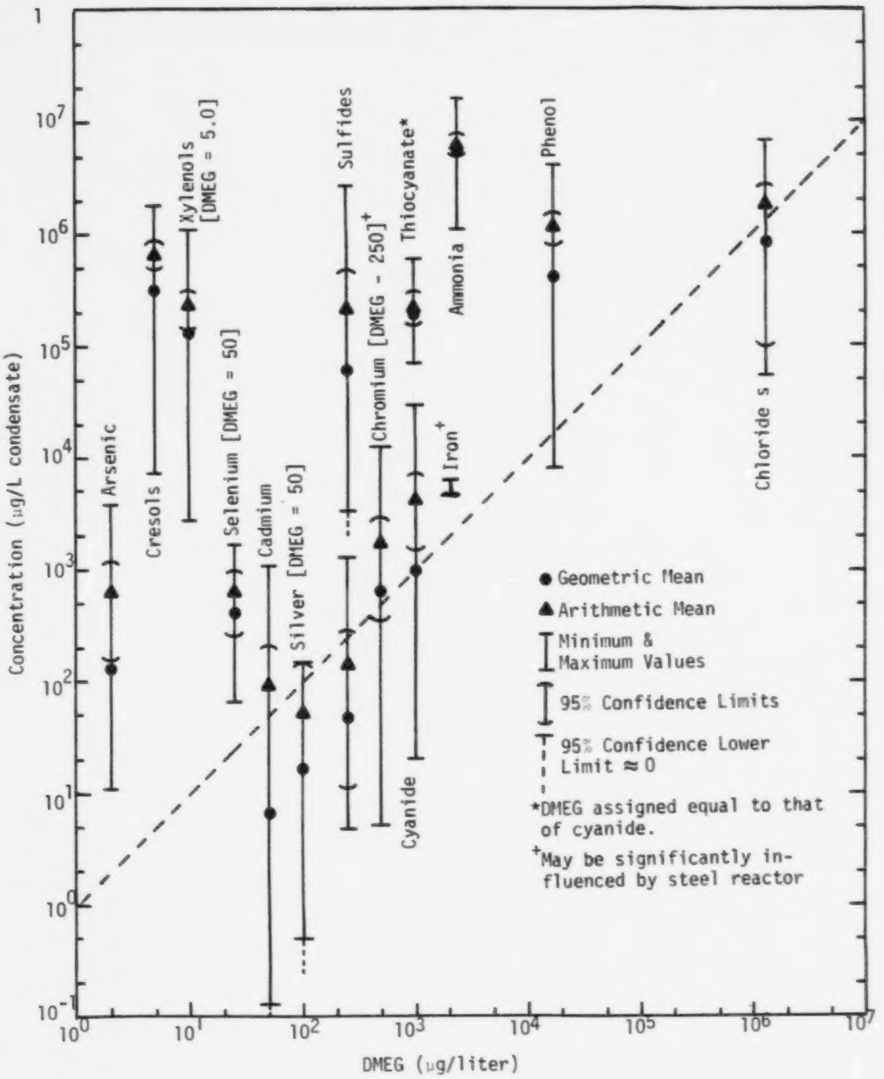

Figure 10. Ranges of concentrations for significant aqueous condensate constituents.

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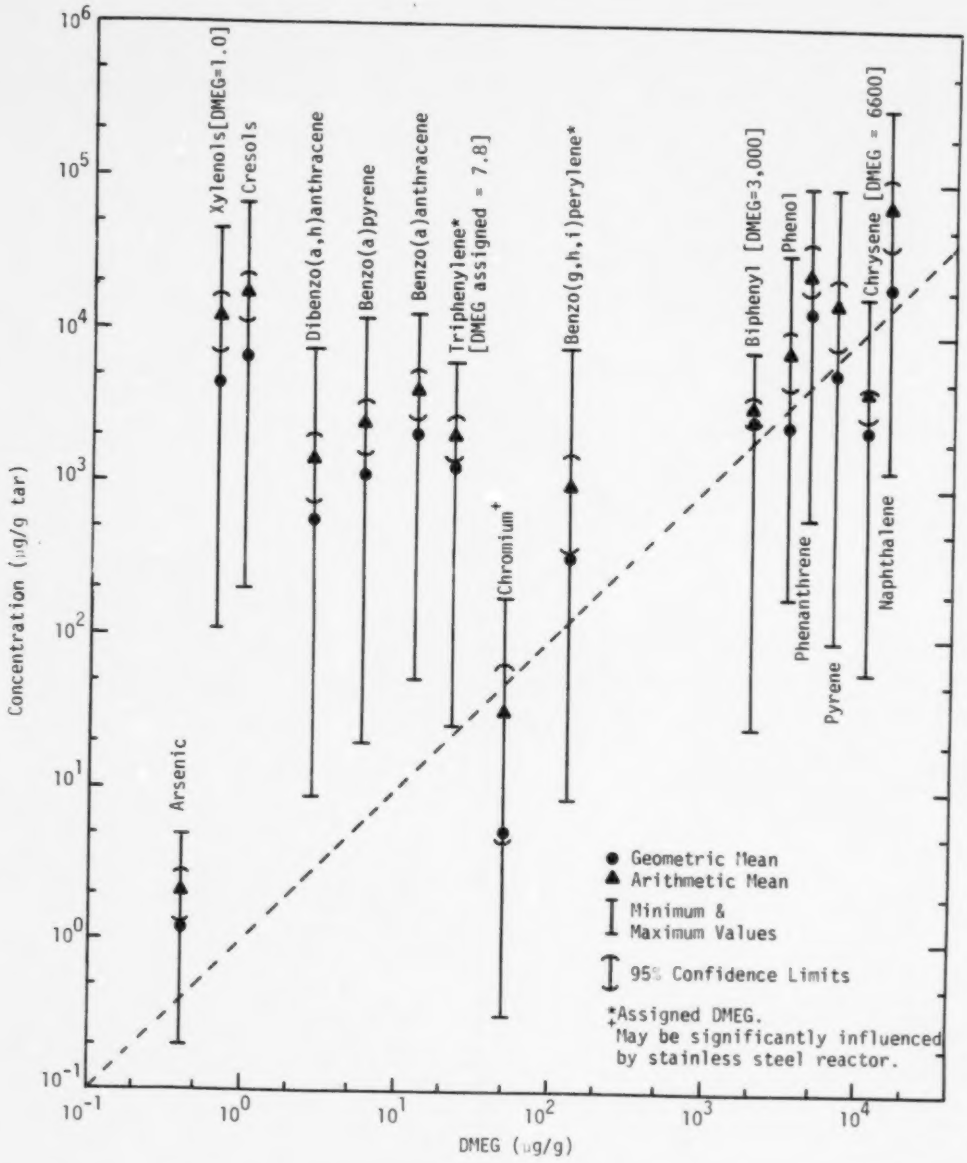

Figure 11. Ranges of concentrations for significant tar constituents.

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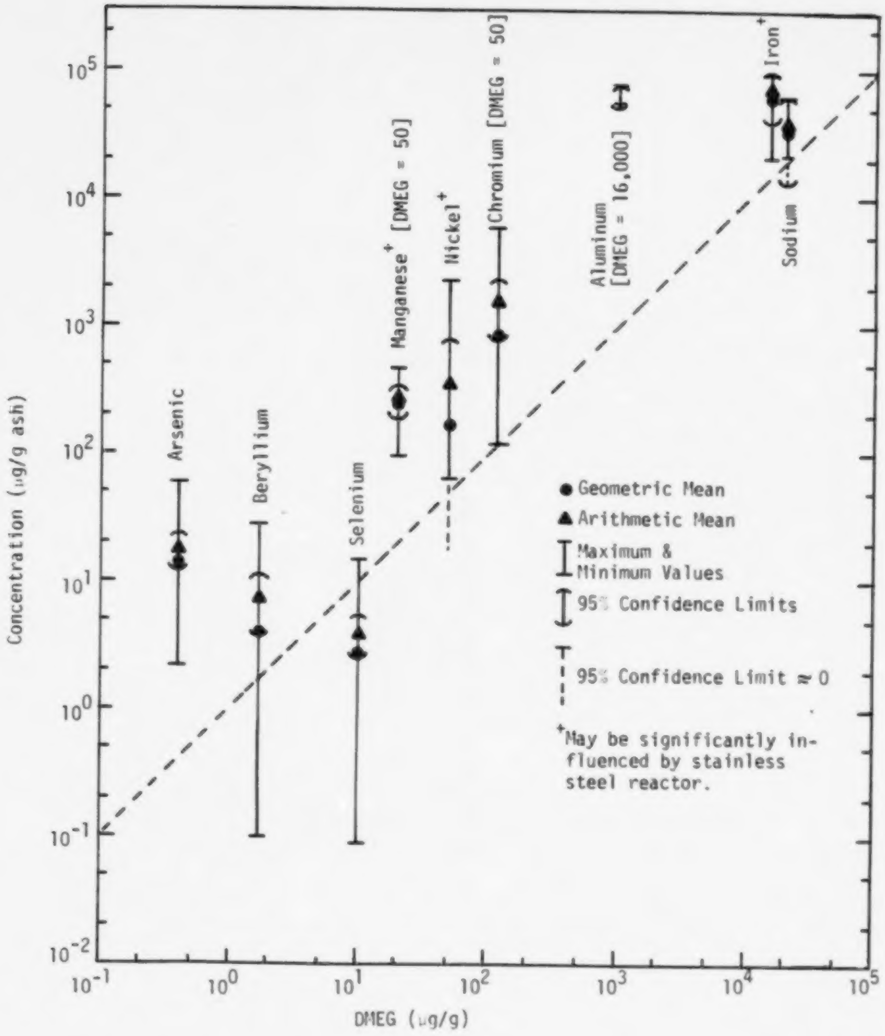

Figure 12. Ranges of concentrations for significant ash elements.

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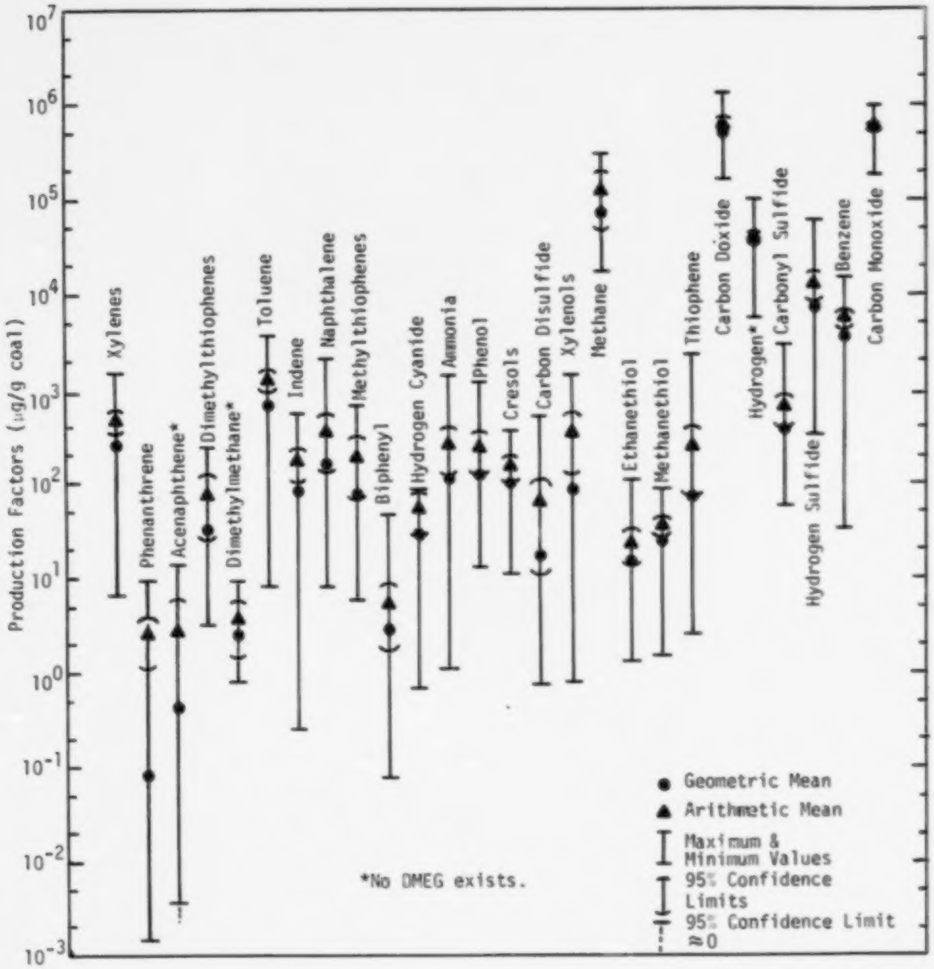

Figure 13. Ranges of production factors for significant product gas constituents.

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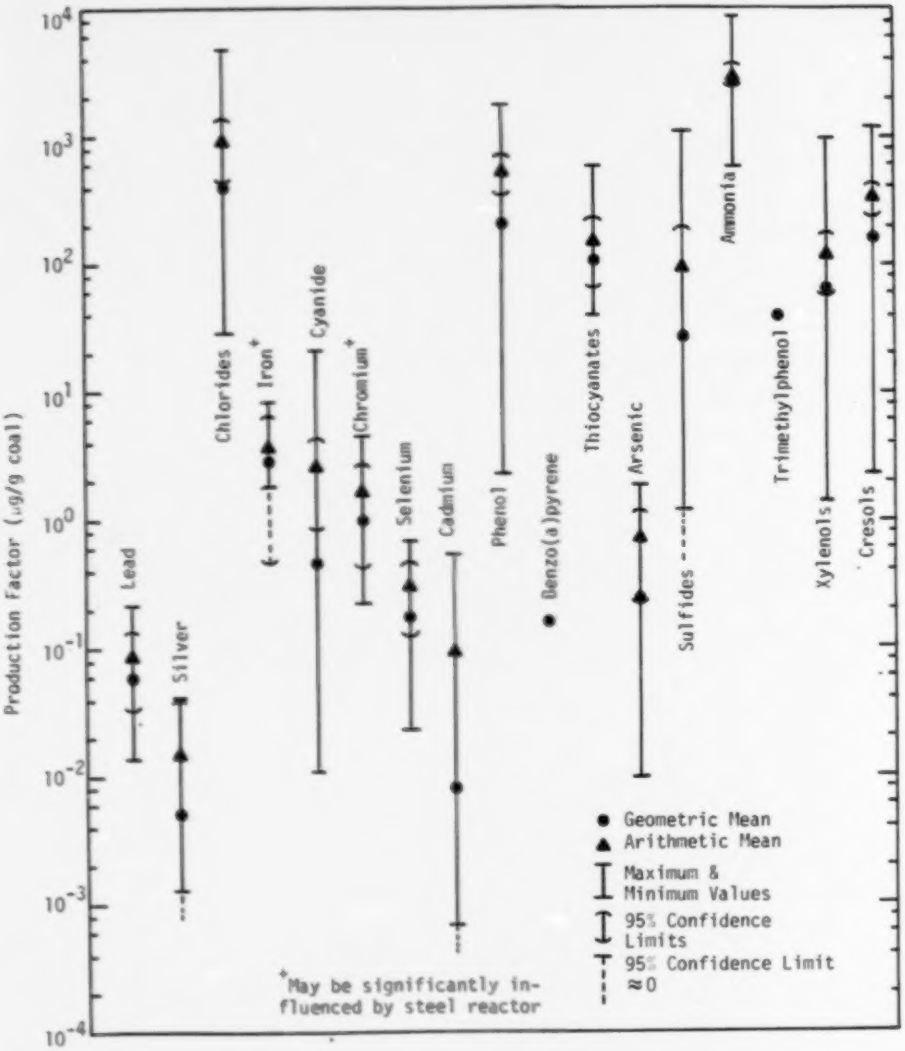

Figure 14. Ranges of production factors for significant aqueous condensate constituents.

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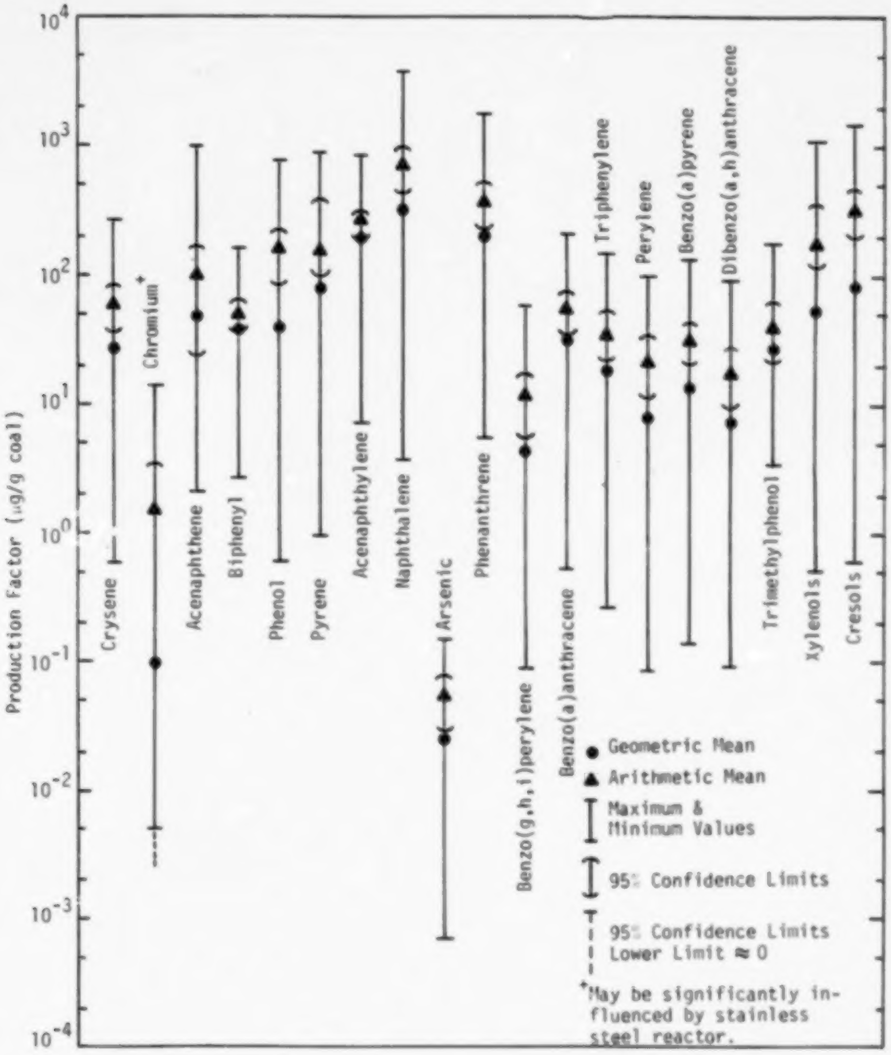

Figure 15. Ranges of production factors for significant tar constituents.

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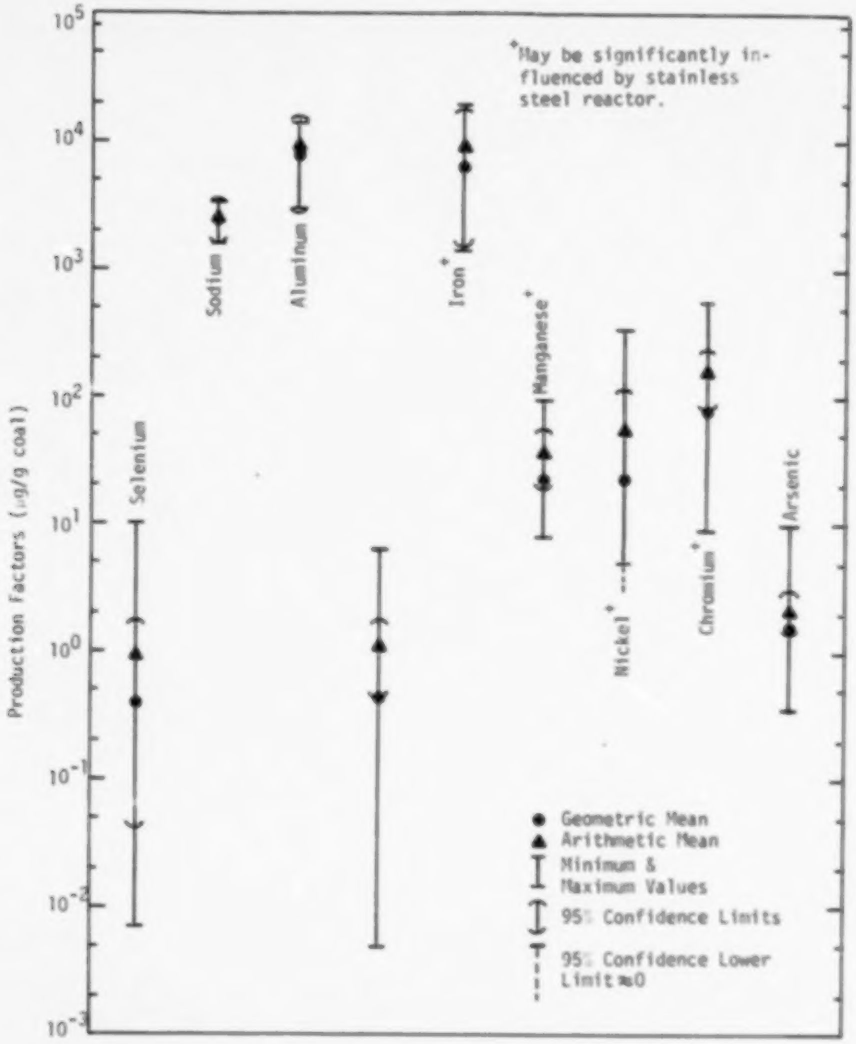

Figure 16. Ranges of production factors for significant ash elements.

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benzo(a)pyrene in tar) per unit weight of coal gasified. Taking crude phenols (phenols, cresols, xylenols) for example, the maximum limit of production from the aqueous condensate is 4000 μg/g which compares favorably to those estimated by C. F. Braun[25] for 1 process with an eastern coal as 3000 μg/g. The ranges of production factors should be useful in obtaining initial material balances; but more importantly; the maximum level should generally be greater or at least equal to those found in commercial processes (see Section 1.0). The concentration and production factor ranges are also useful (in addition to their uses of determining pollutant significance, efficiency of control device needed, etc.) to enable chemists to calibrate their analytical instruments in future studies of pollutant generation from coal gasification.

5.2.2 Control Priority

Another concept of interest in environmental assessment is that of control priority. This concept, originally called minimum diluent for process stream and introduced by Cleland and Pierce,[26] is a convenient way to measure the need to control various pollutants in the individual streams. It complements the discharge severity concept in that it determines how much air, water, or land are required per unit amount of coal gasified to dilute the stream with respect to a particular pollutant to bring the level down to a nonhazardous level. Control priority is defined as

$$\text{Control priority} = \frac{\text{Production Factor}}{\text{DMEG}} . \qquad (3)$$

Thus, the unit of control priority for the gas pollutants is m^3/g coal; for the aqueous condensate pollutants; it is L/g coal and for tar and ash streams, it is g/g coal. It indicates the m^3 of air, the liters of pure water, or the grams of land needed to dilute the effluent stream to make it nonhazardous with respect to a pollutant. Control priority is thus a measure of need to control and is especially useful in obtaining an overall stream dilution necessary (see Section 5.3). Control priority for significant constituents in the four streams are shown in Figures 17, 18, 19, and 20 for gas, aqueous condensate, tar, and ash, respectively. The constituents are listed from left to right in decreasing order of discharge severity.

5.3 TOTAL STREAM EVALUATION

Gross effluent stream amounts per unit weight of coal gasified are presented in Table 14. Arithmetic and geometric means, standard deviation, minimum, maximum, and 95 percent confidence interval of the effluent stream amounts for some 30 gasification tests are depicted in this table. To put an environmental perspective on the effluent streams, let us consider a large-scale low-Btu coal gasification facility processing some 15000 t/day of coal. Assuming that it would produce, on the average, effluent streams corresponding to the arithmetic mean in Table 14, one would have to process and/or contain on a yearly (365 days) basis some 1.0 billion gallons of aqueous condensate, 1.0 billion tons of ash, and 0.1 billion tons of tar.

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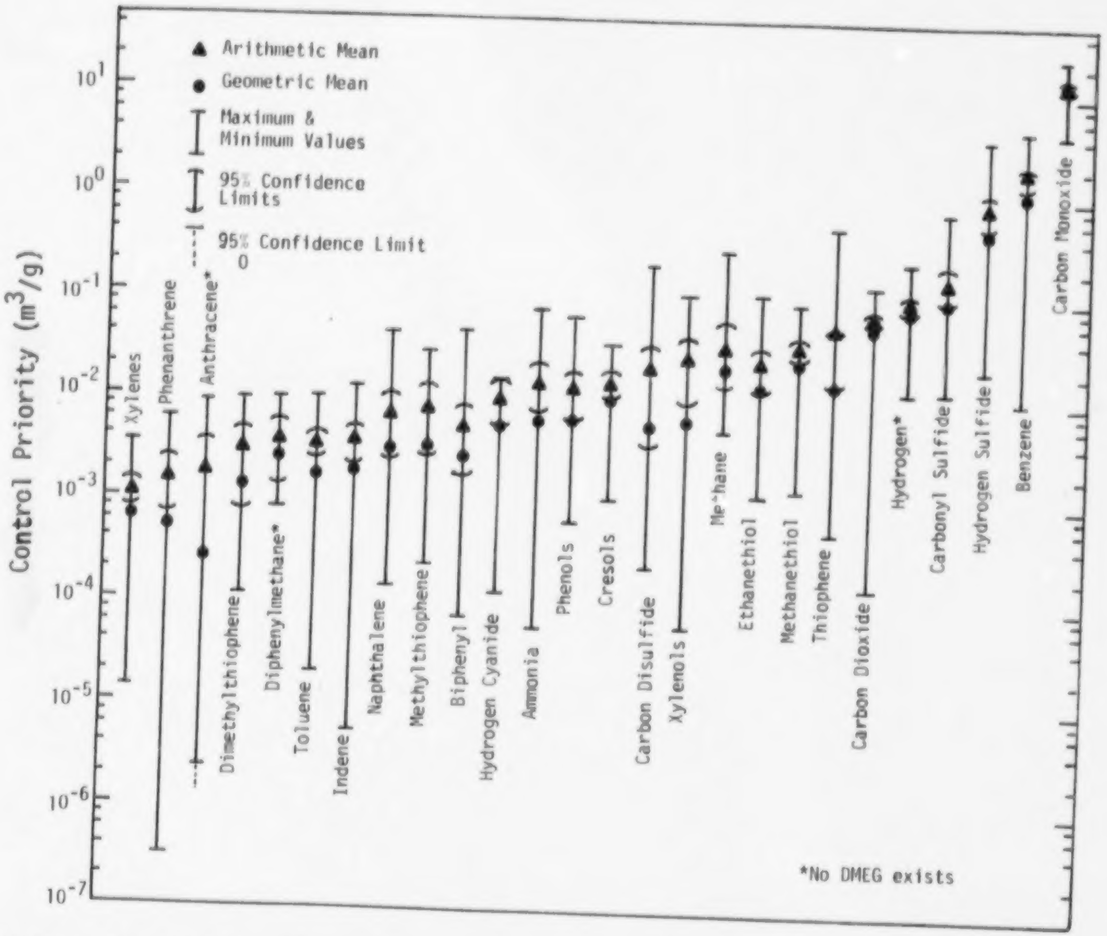

Figure 17. Ranges of control priorities for significant product gas constituents.

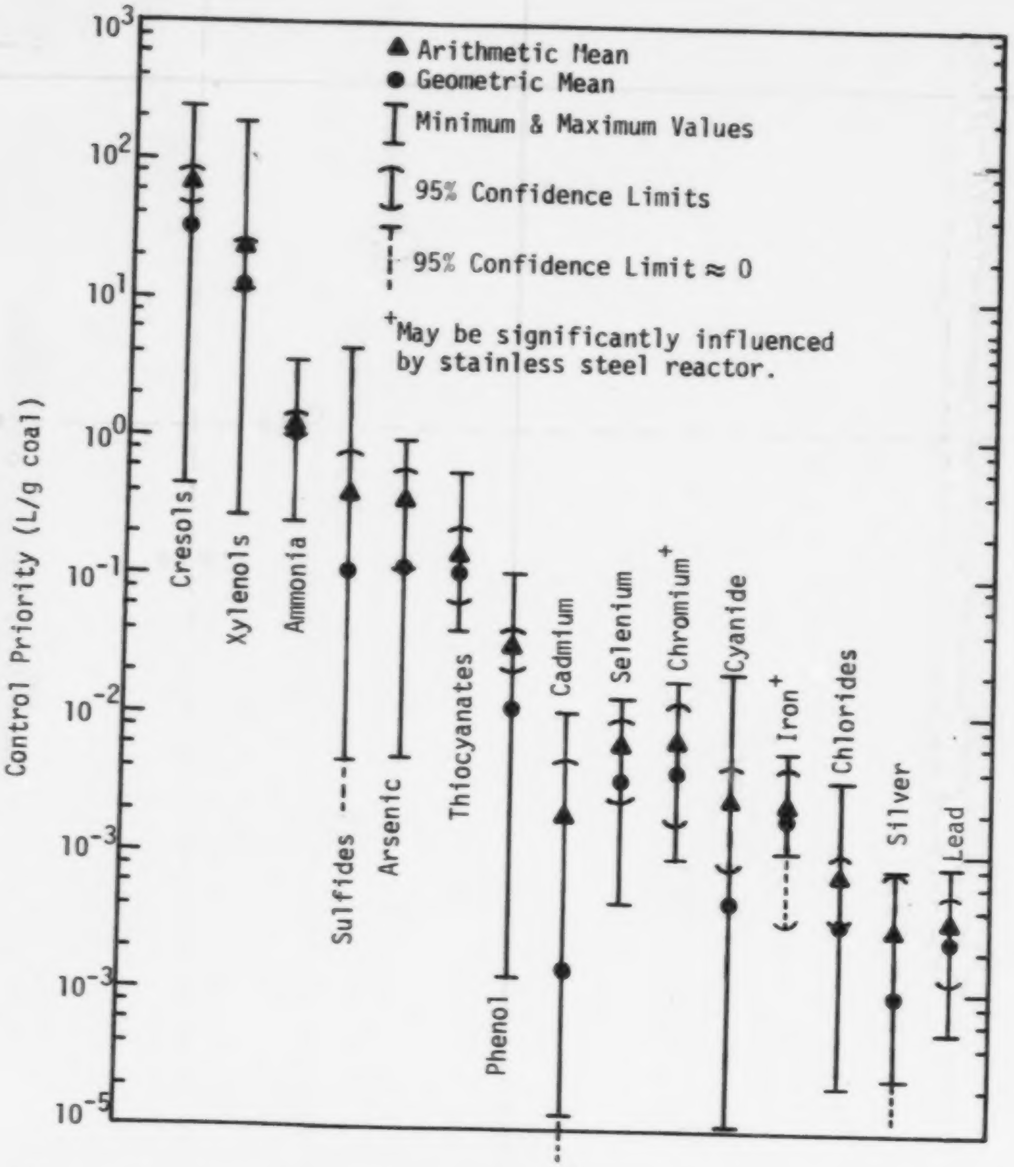

Figure 18. Ranges of control priorities for significant aqueous condensate constituents.

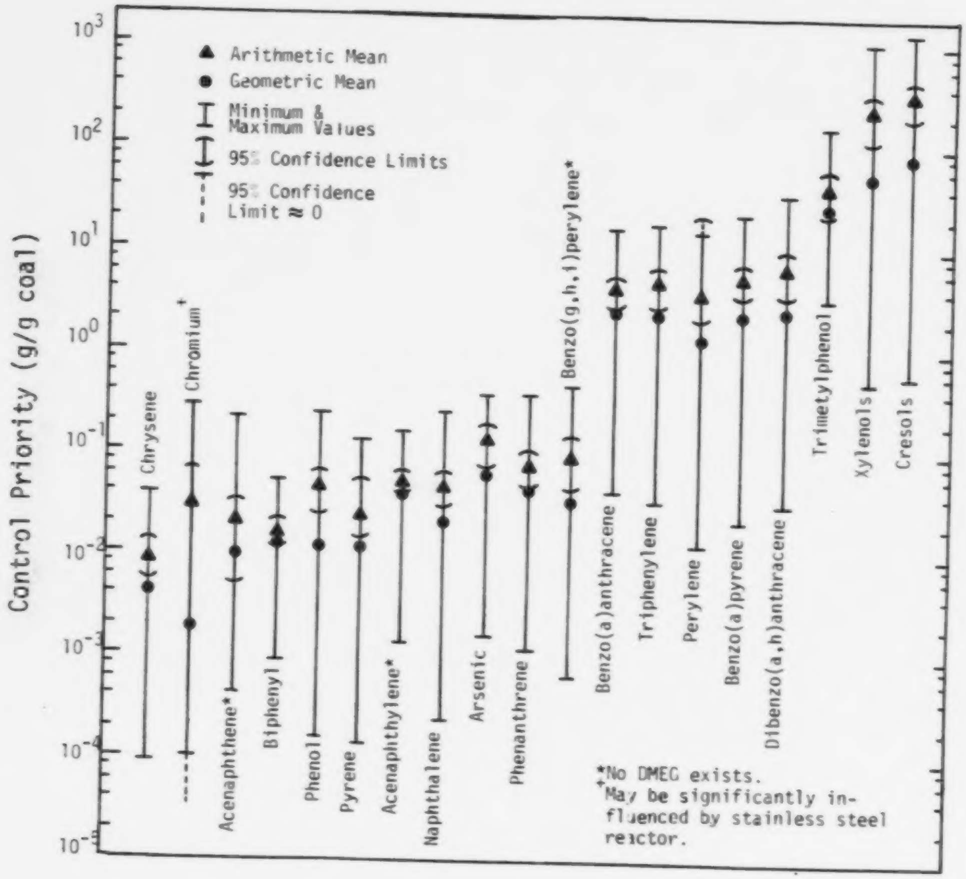

Figure 19. Ranges of control priorities for significant tar constituents.

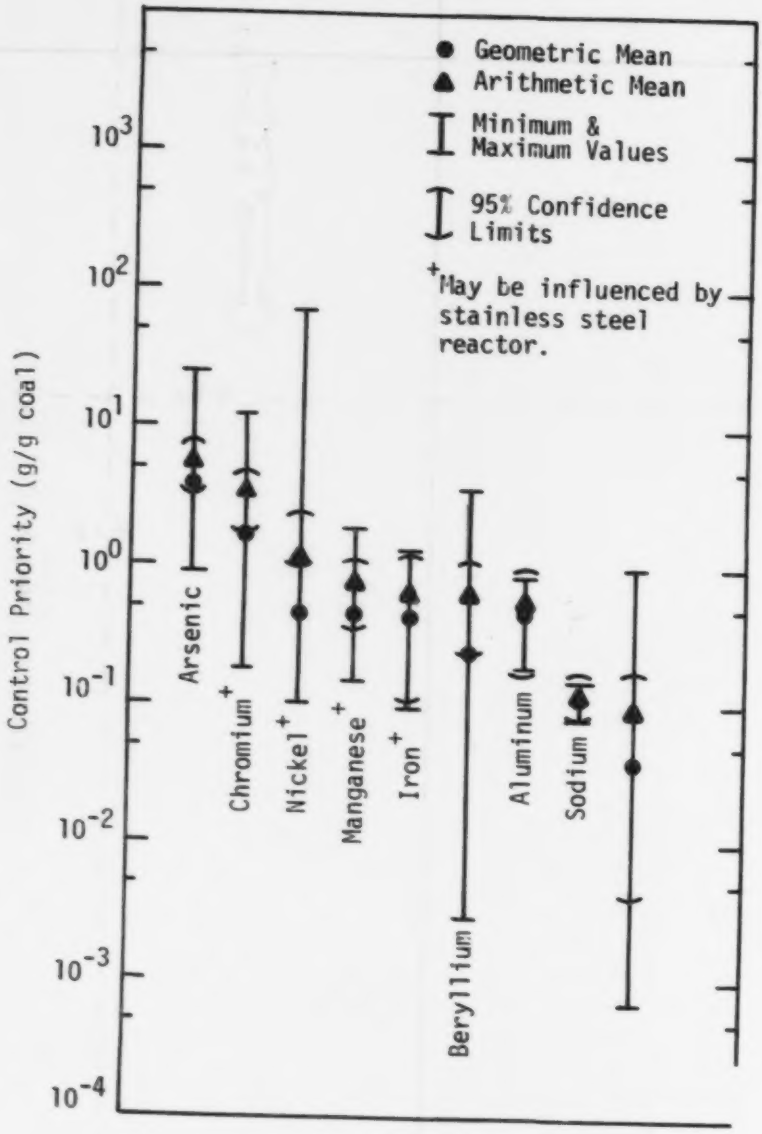

Figure 20. Ranges of control priorities for significant ash elements.

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TABLE 14. GROSS EFFLUENT STREAM AMOUNTS PER UNIT OF COAL

Stream	Units/gram of Coal	No. of Tests	Geometric Mean	Arithmetic Mean	Standard Deviation	Minimum	Maximum	95% Confidence Lower Bound	95% Confidence Upper Bound
Gas	Std. Liters	34	2.6	2.7	0.8	1.5	4.7	2.4	3.0
Aqueous Condensate	ml	36	0.57	0.81	0.98	0.12	5.8	0.49	1.1
Tar	mg	35	14	19	13	1.4	56	15	23
Ash	g	27	0.15	0.20	0.17	0.04	0.74	0.14	0.26

In order to evaluate the total and relative stream hazard factors, three distinct approaches were taken, based on summing up hazards from individual pollutants. These approaches are summarized in Table 15.

From the stream discharge severity (first row), aqueous condensate and tar are seen to be the most severe streams. This is primarily caused due to the dominance of cresols and xylenols. Recently DMEG for phenol was increased almost three orders of magnitude, thus it seems unreasonable to keep the DMEG for cresols and xylenols lower. By assuming that DMEG of cresols and xylenols equals that of phenol the stream discharge severities reduces to 8,000 for aqueous condensate and 5,000 for tar. For product gas, most of the severity is contributed by CO (about 6,000 out of 7,000), a product that one is trying to maximize. The ash appears to be relatively nonhazardous. These points are further discussed in Section 6.0 where comparison is made of RTI gasifier effluents to those from other processes.

Overall control priorities are calculated as follows. The mean stream production factor is divided by the stream DMEG and summed for individual pollutants. Thus, one sees that on the average, one needs some 20 m^3 of air, 100 liters of water, and 700 grams of land to dilute the gas, aqueous condensate, and the tar streams, respectively, for every gram of coal gasified. The ash again appears relatively nonhazardous, needing only 10 grams land dilution per gram of coal gasified. The hazard associated with various streams is discussed further in Section 5.4 where bioassay results show tar to be the most mutagenic and toxic among the various streams.

5.4 BIOASSAY RESULTS

The bioassay studies which have been conducted include both the Ames mutagenicity assay and the Chinese hamster ovary cell cytotoxicity assay in both the growth kinetics and clonal efficiency modes. These were described in Section 4.2. The samples which were tested include raw coal dusts, aqueous condensate, XAD-2^R resin, and crude tars and its fractions. These results were discussed in detail in an earlier report.[4] However, some recent results on tars which were not reported earlier showed interesting differences from those reported earlier.

Briefly, the findings from the earlier study[4] indicated that raw coal dusts from North Dakota lignite, Wyoming subbituminous, Western Kentucky No.9, and Illinois No.6 tested negative for mutagenic activity using the Ames test as well as negative for cytotoxicity using the CHO growth kinetics and clonal efficiency assays. The aqueous condensate samples tested negative to the Ames test and only showed a marginal influence on CHO cells. The XAD-2 samples tested negative to the Ames test but showed significant cytotoxicity in the growth kinetics test (the results of the clonal efficiency test were inconclusive since XAD-2 control showed similar cytotoxicity as the XAD-2 samples). The most interesting result of the earlier study was obtained with bioassay on crude tars and its fractions. As stated in Section 2.3, the crude tars from every gasification test were subjected to a solvent partitioning scheme. This resulted in six fractions. These are polar neutrals, polynuclear aromatics, nonpolar neutrals, cyclohexane

TABLE 15. OVERALL STREAM EVALUATION BASED ON MEAN POLLUTANT CONCENTRATIONS

	Units	Summation Formulas	Gas	Aqueous Condensate	Tar	Ash
Stream Discharge Severity	None	$\sum_i \frac{\bar{C}_i}{DMEG_i}$	7×10^3	2×10^5	3×10^4	100
Stream Control Priority	+	$\sum_i \frac{\bar{PF}_i}{DMEG_i}$	20	100	100	10

+Units for gas = m^3/g, aqueous condensate = L/g, tar and ash = g/g.

insolubles, acids, and bases. Ranges of these fractions in all gasification tests including arithmetic and geometric means, minimum, maximum, and 95 percent confidence intervals are shown in Figure 21.

It was seen from the bioassay tests that the crude tar samples and many of the fractions exhibited both strong cytotoxicity as well as mutagenicity. The highest responses in the CHO growth kinetics assay resulted from both crude tars and their partition fractions, including the organic bases, PNAs, polar neutrals, and, in some cases, the organic acid fractions. Similar results were obtained for the clonal efficiency assay. The crude tar samples from Illinois No.6 and Western Kentucky No.9 coal gasification runs were found to possess the same level of cytotoxicity per unit mass as was exhibited by the combination of their partition fractions. However, the crude tar sample from the Wyoming subbituminous gasification run was substantially less cytotoxic per unit mass than its partition fraction equivalent. This phenomenon is referred to here as an "unmasking effect" where the fractions either add up to or individually possess higher activity. For the Illinois No.6 coal, the nonpolar neutral and PNA fractions exhibited high cytotoxicity; for the Western Kentucky No.9 coal, the organic bases, organic acids, and PNAs were found to be most cytotoxic; while for the Wyoming subbituminous coal, the PNAs, organic acids, and polar neutrals exhibited greatest cytotoxicity.

All these earlier studies are reported in full detail.[4] The tars that were examined in these studies were generated in batch gasification runs. Recently, as stated in Section 2.1, the gasifier has also been operated in the continuous feed mode. Interestingly, various tars and their fractions exhibited weaker mutagenicity for these continuous feed runs compared to the batch runs. Comparison of the mutagenicity of the batch run tars and their fractions versus the continuous run tars are shown in Figures 22, 23, and 24. From Figure 22, the continuous run tar, base, and PNA fractions for Wyoming coal were significantly less mutagenic than those for the batch run. On the other hand, even though the base fraction for the semibatch North Dakota lignite run (Figure 23) was substantially more mutagenic than the continuous run, the crude tar itself and the PNA fraction in both cases were similar and weakly mutagenic. For Illinois No.6 coal, both the base and the PNA fractions are strongly mutagenic for the semibatch run, but the tar is apparently so toxic that it is not possible to get a good result for the mutagenicity. For the continuous runs (C6 and C7), tar is only weakly mutagenic. Unfortunately, the base fraction of the continuous run, Illinois No.6 coal, tar was not tested for mutagenicity, but concluding from results of the Wyoming and North Dakota tars, it would be expected to have lower mutagenicity than the semibatch tar.

Now the question is, why are the continuous run tar base samples much less mutagenic than the semibatch run tar base samples? The answer is obviously tied up in the chemical constituents of the two samples. A detailed chemical analysis of the Wyoming subbituminous and North Dakota lignite tars showed that the continuous run tars had a much greater proportion of parent compounds compared to the semibatch run tars. These results are reported in detail by Gangwal and Nichols.[20] Here parent

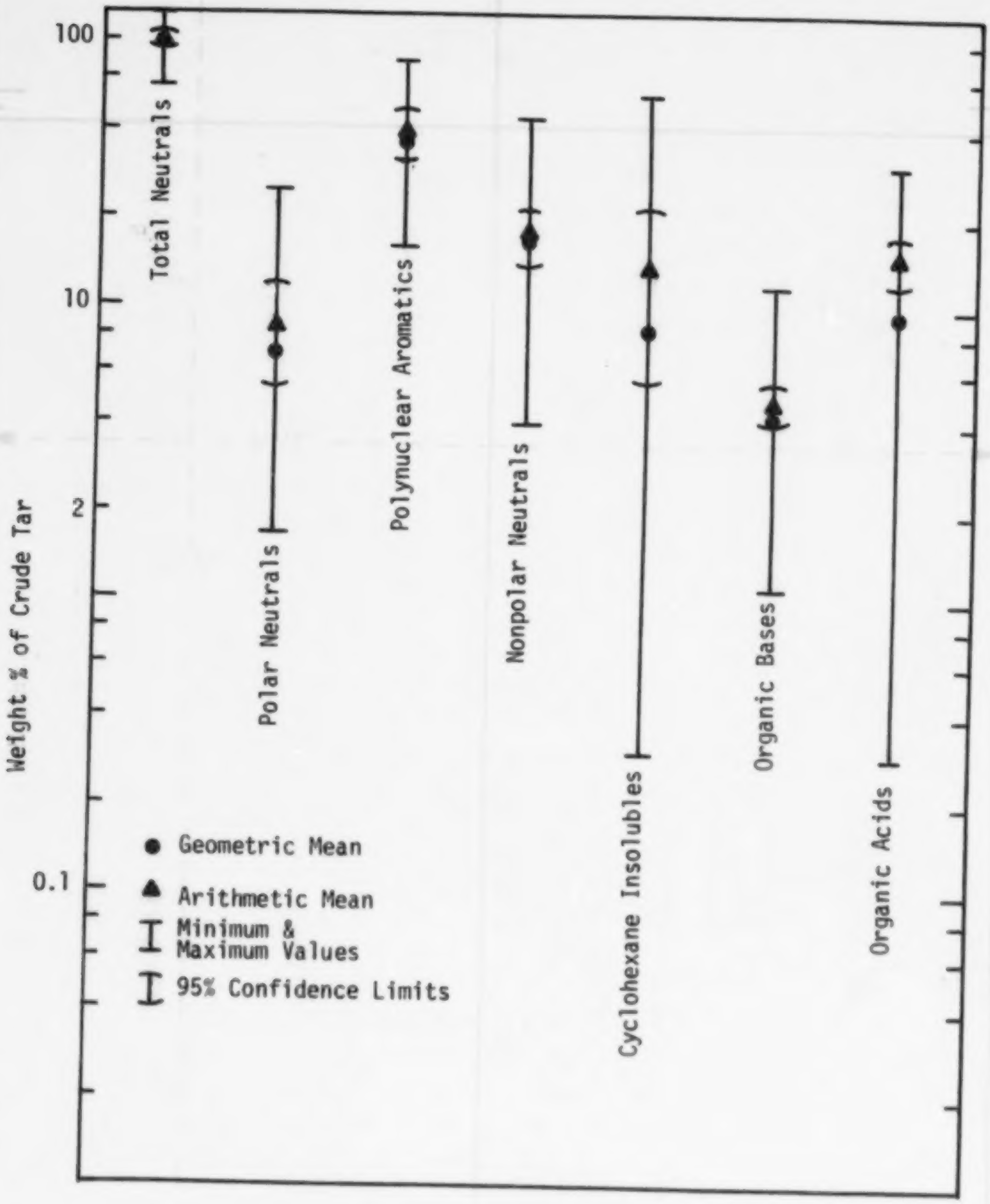

Figure 21. Ranges of tar partition fractions as weight percent of crude tar.

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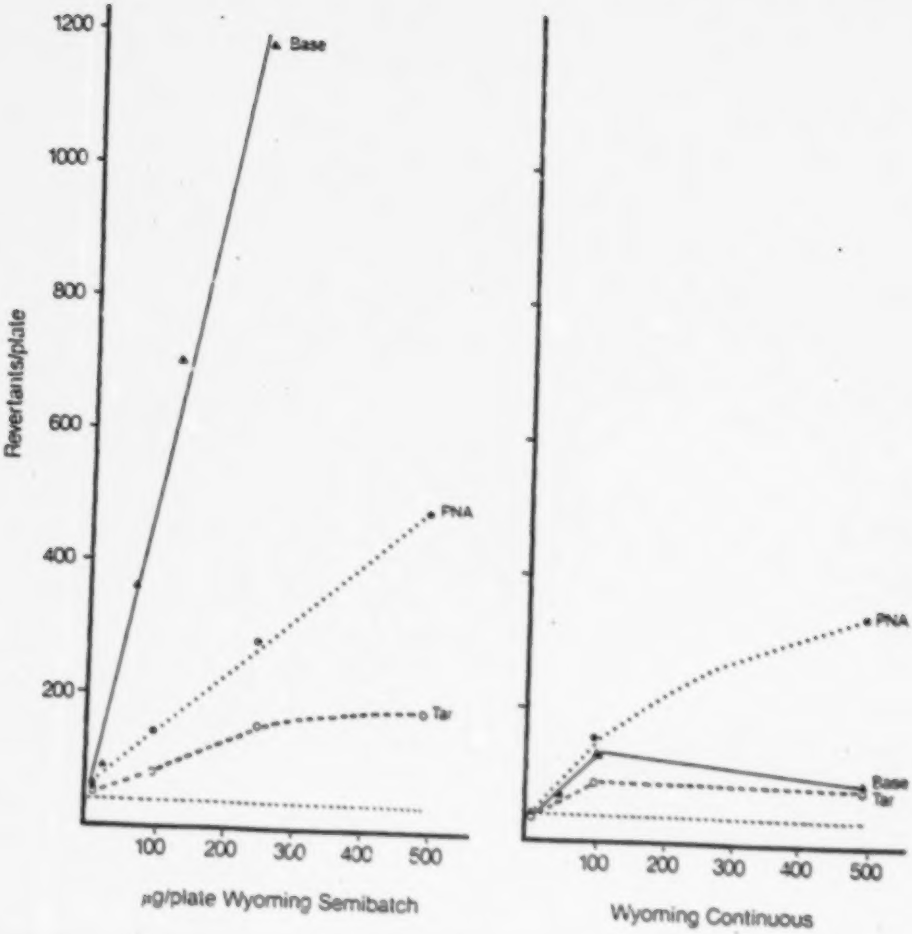

Figure 22. Comparison of mutagenicities for Wyoming semibatch tar and its fractions to those for Wyoming continuous tar and its fractions.

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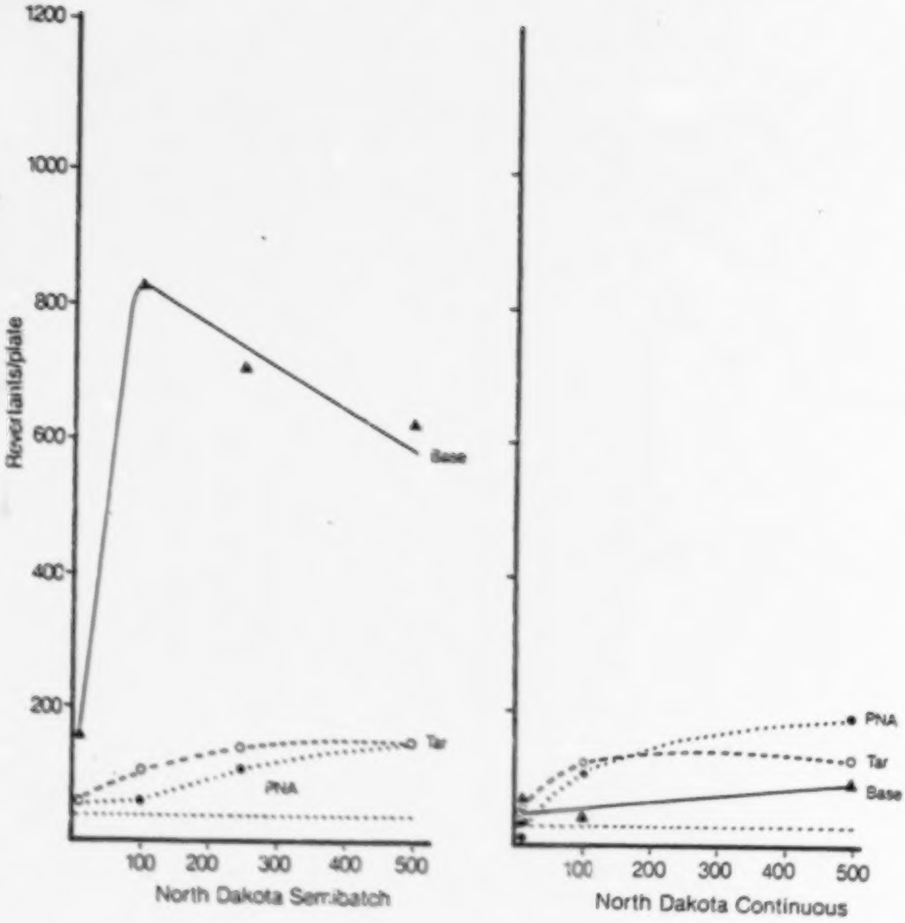

Figure 23. Comparison of mutagenicities for North Dakota semibatch tar and its fractions to those for North Dakota continuous tar and its fractions.

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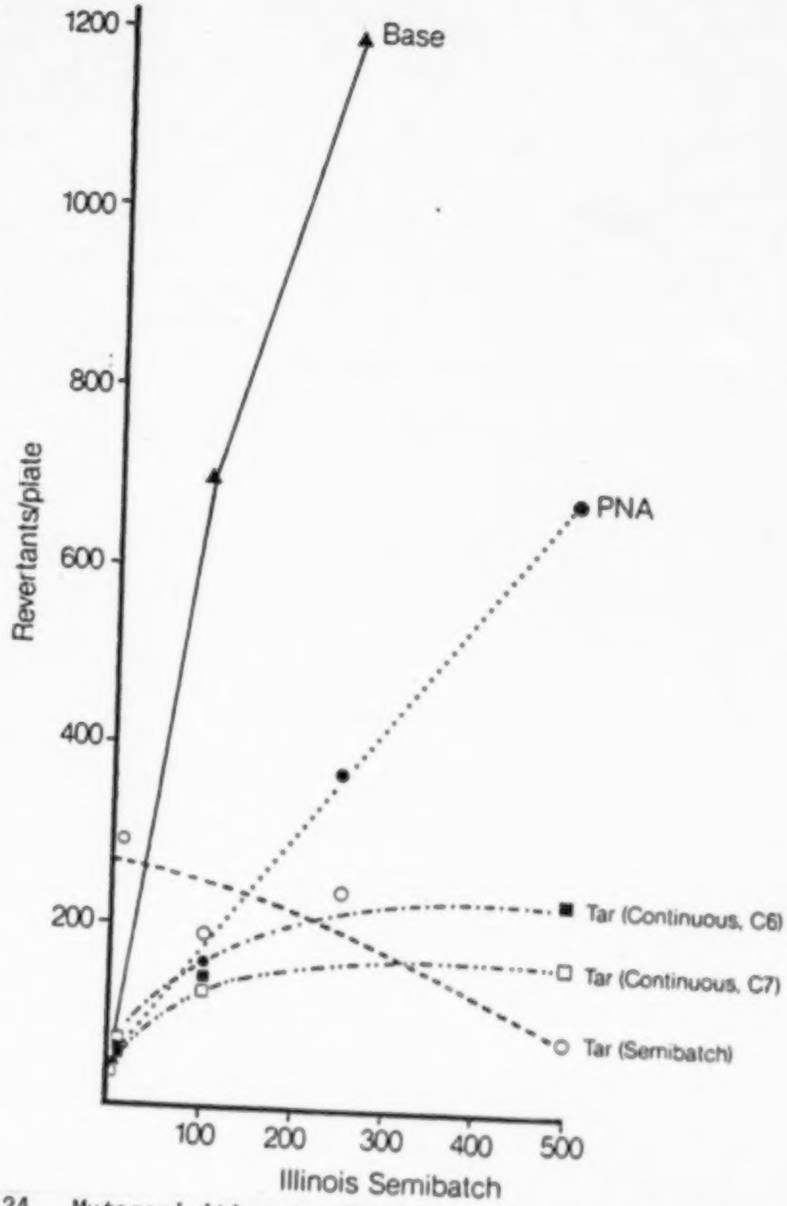

Figure 24. Mutagenicities for Illinois semibatch and continuous tars and semibatch tar fractions.

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compounds are compounds such as naphthalene, phenanthrene, fluoranthene, etc. The continuous run tars had a significantly lower proportion by weight of compounds with side chains. Thus, one hypothesis is that some of these branched chain compounds are the ones which most likely impart severe mutagenicity to the tar base fractions. Some of the most potent mutagens known to date are aromatic amines.[11] Aminonaphthalenes quantitated for the continuous run tars are consistently below the DMEG and were in fact eliminated (see Table 4). Unfortunately, semibatch run tars were not analyzed for aminonaphthalenes but there is a general agreement between various research groups that in fact these amino compounds are responsible for the mutagenicity and the data reported here do not refute this view since the continuous run tar bases with insignificant amounts of aminonaphthalenes were also weakly mutagenic. The continuous feed mode apparently pyrolyzes coal at a higher temperature than the batch mode. Also the reactor itself stays hotter, thereby increasing the cracking rates of these compounds with side chains. Thus, one sees less tar (since the side chain aromatics are reduced) and a greater proportion of parent compounds (which crack to a lesser degree) in the tar for continuous runs.

6.0 DISCUSSION

A laboratory coal gasification facility has been employed to evaluate relative environmental hazards of effluent streams (namely gas, aqueous condensate, tar and ash) and their constituents. The procedure included:

1. Gasification of a variety of coals under a variety of conditions.
2. Extensive chemical analyses of effluent streams.
3. Application of MEG methodology for (a) elimination of insignificant pollutants, (b) determination of discharge severities of significant pollutants, and (c) overall stream hazard evaluation.

The results of this study were presented in detail in Section 5.0. These are discussed here further especially in relation to those obtained by other research groups on other large-scale gasifiers and processes. Discussion of methods and results on overall and individual streams follows.

6.1 OVERALL STREAM COMPARISONS

The relative hazards from the RTI gasifier for individual streams, i.e., gas, aqueous condensate, tar, and ash were discussed in Section 5.3. Here, comparisons are made for these streams with those obtained from large-scale gasifiers (Table 16). The aqueous condensate production is greatly influenced by the gas cooling process imposed and end use. Thus the Wellman-Galusha process produces no condensate because the entire hot gas is combusted. Thus, any moisture would end up in the combustion flue gas. The Chapman-Wilputte process uses an evaporator system, and no condensate is discharged as liquid. No tars are produced from the Wellman-Galusha and the Koppers-Totzek gasifiers because the former uses an anthracite coal and the latter is an oxygen-blown entrained-bed process. For the air-blown gasifiers, RTI gas production appears to be low presumably because of a lower throughput in the laboratory reactor. Ash is influenced by coal type, but in general the RTI range compares favorably to other gasifiers. Tar production compares favorably to METC, GFETC, and Lurgi but not to Chapman-Wilputte.

6.2 PRODUCT GAS

The chemical analysis methods for product gas were relatively straightforward with a few exceptions noted in Section 2.3. Some 26 constituents in the gas phase exceeded their DMEG (see Table 6) but only carbon monoxide, benzene, hydrogen sulfide, and carbonyl sulfide appear to be of major environmental concern (mean DS exceeds 50), as seen in Table 10. Almost 98 percent of the overall discharge severity is contributed by these four

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TABLE 16. COMPARISON OF EFFLUENT STREAM PRODUCTION FROM DIFFERENT GASIFIERS

	95% Confidence Range (This Study)	Chapman Wilputte[27]	Wellman Galusha[28] (Anthracite Coal)	METC[29]	GFETC[30] (Oxygen blown)	Lurgi[31] (Oxygen blown)	Koppers Totzek[32] (Oxygen Blown)
Gas m^3/kg coal	2.4-3.0	2.9	5.4	2.8-6.0	0.98-1.1	1.2	2.0
Aqueous Condensate L/kg coal	0.49-1.1	0	0	1.5-4.9	0.2-0.33	0.82	0.22
Tar g/kg coal	15-23	100	0	11-47	16-23	21	0
Ash kg/kg coal	0.14-0.26	0.06	0.9	0.07-0.18	0.06-0.07	0.18	0.24

compounds. Furthermore, both carbon monoxide and benzene are valuable products from coal gasification. Ranges of concentrations and production factors are shown in Figures 8, 9, and 13. A maximum variation of three orders of magnitude is seen. The fixed gases (CO, CO_2, H_2 and CH_4) show the least variability as a function of coal type and process conditions. Considering the 95 percent confidence interval around the arithmetic mean as the most likely range, the maximum variation reduces to substantially less than one order of magnitude for all significant constituents.

Comparison of the laboratory gasifier product gas to those obtained from other gasifiers is shown in Table 17 for various significant constituents. The 95 percent confidence interval of concentrations for the laboratory gasifier compares quite favorably to values for larger scale gasifiers, especially the low-Btu gasifiers.

This lends credence to the RTI gasifier in its ability to simulate large-scale processes with respect to both pollutant production as well as production of major gas constituents. The only constituent for which the RTI gas concentration appears low in comparison to other gasifiers is ammonia. This may be caused due to low scrubber efficiency for ammonia capture. Fortunately, the majority of the ammonia condenses out as aqueous ammonia in the condensate (see Section 6.3) and thus the low gas value introduces little error to overall ammonia production. Also adequate comparison with other gasifiers are difficult, because of differences in condensation or quench temperatures and procedures.

Further, comparisons of the gas stream with U.S. ambient air, urban, and nonurban background concentrations, and NIOSH recommended exposure limit are shown in Table 18. For comparison of gasification with combustion, data from processes such as fluidized bed combustion and residential coal-burning are also included. From Table 17, gasifier gas has CO concentrations almost four orders of magnitude greater than the NIOSH-recommended standard; thus, CO again appears to be the greatest gas hazard. Another point of interest is that the mean methanethiol level is in fact lower than the current Federal occupational standard. The PAHs quantitated are generally orders of magnitude greater than background concentrations, and benzene, toluene, xylenes, cresols, and phenols are individually almost six orders of magnitude greater. Comparing to combustion, fluid bed combustion produces flue gas of very low PAH content, whereas residential coal furnace produced greater amounts of gas phase PAHs than gasification.

6.3 AQUEOUS CONDENSATE

Procedures for the analysis of aqueous condensate were discussed in Section 2.3. Briefly, the aqueous condensate was analyzed for various constituents using HPLC, GC-MS, and standard wet chemical techniques and for trace elements using atomic absorption spectrometry (AA) and neutron activation analysis (NAA). Trace organics, including PAHs, were analyzed for in one aqueous sample using a methylene chloride extraction followed by glass capillary gas chromatography (GC^2). Sixteen constituents in the aqueous phase exceeded their DMEG (see Table 7). Of these, nine compounds appear to

TABLE 17. COMPARISON OF CONCENTRATIONS $[\mu g/m^3]$ AND PRODUCTION FACTORS $[\mu g/g$ coal$]$[†] OF SIGNIFICANT PRODUCT GAS CONSTITUENTS FROM DIFFERENT GASIFIERS

	95% Confidence Ranges for This Study	METC[29] (Average for 7 Coals)	Range (3 Coals) Air-Blown Synthane[33]	Wellman-Galusha[28] (Penn.-Anthr. Coal)	Koppers-Totzek[34] (Oxygen-Blown)	Dry Ash[34] Lurgi
Carbon Monoxide	2.0E8-2.8E8	2.6E8	1.3E8-2.0E8	--	7.3E8	--
Benzene	1.6E6-2.6E6 (4.2E3-7.0E3)	--	2.4E6-3.4E6 (4.8E3-7.4E3)	--	--	
Hydrogen Sulfide	3.0E6-6.0E6 (8.4E3-1.8E4)	5.5E6	8.8E5-7.6E6 (2.0E3-1.3E4)	8.9E5 (4.9E3)	4.3E6-2.6E7 (6.6E3-4.6E4)	6.7E6 (9.6E3)
Carbonyl Sulfide	1.4E5-2.8E5 (3.8E2-8.8E2)	--	5.4E4-3.8E5 (1.2E2-7.6E2)	2.2E5 (1.2E3)	5.5E5-1.8E6 (8.0E2-3.2E3)	--
Hydrogen	1.2E7-1.8E7	1.3E7	2.0E7-2.7E7	--	2.9E7	--
Carbon Dioxide	2.2E8-2.8E8	1.9E8	3.7E8-3.8E8	--	2.1E8	--
Thiophene	2.9E4-1.3E5 (7.0E1-4.1E2)		<1.9E4-2.6E5 (<3.8E1-4.4E2)	--	--	--
Methanethiol	1.0E4-1.8E4 (2.6E1-4.4E1)	--	1.7E4-8.6E4 (3.4E1-1.5E2)	-- --	-- --	-- --
Methane	2.1E7-3.1E7	1.8E7	3.1E7-4.0E7	--	0-8.3E5	--
Ammonia	4.9E4-1.3E5 (1.2E2-4.0E2)	--	--	1.2E5 (6.9E2)	--	--
Toluene	3.9E5-2.5E5 (9.4E2-1.7E3)	--	2.9E5-9.0E5 (5.8E2-1.8E3)	--	--	--
Xylenes	1.3E5-6.9E5 (3.4E2-6.2E2)	--	9.5E4-2.8E5 (1.9E2-6.2E2)	--	--	--

continued

[†] Production factors in parenthesis.

--Blanks in table indicate values not available.

TABLE 17 (continued).

	95% Confidence Range for This Study	Bigas[34]	GFETC[34,35] (Oxygen Blown)	CO_2[34] Acceptor	Chapman[27] Wilputte	Woodall[35] Duckham	Winkler[35]	Lurgi[34] (Oxygen Blown-Range for 5 Coals)
Carbon Monoxide	2.0E8-2.8E8	2.8E8	7.5E8	--	2.6E8	3.7E7	2.9E8	2.0E8-2.7E8
Benzene	1.6E6-2.6E6 (4.2E3-7.0E3)	--	--	--	--	--	--	--
Hydrogen Sulfide	3.0E6-6.0E6 (8.4E3-1.8E4)	8.5E6 (3.9E4)	8.7E5 (1.5E3)	1.6E6 (2.1E3)	4.0E5	--	--	7.0E6-1.6E7
Carbonyl Sulfide	1.4E5-2.8E5 (3.8E2-8.8E2)	3.0E6* (1.3E4)*	7.6E4* (1.3E2)*	7.4E4 (9.7E1)	--	--	--	--
Hydrogen	1.2E7-1.8E7	1.4E7	2.8E7	--	1.4E7	1.6E7	1.3E7	3.7E7-3.9E7
Carbon Dioxide	2.2E8-2.8E8	1.5E8	1.6E8	--	1.8E8	3.7E8	1.5E8	6.0E8-6.5E8
Thiophene	2.9E4-1.3E5 (7.0E1-4.1E2)	--	--	--	--	--	--	--
Methanethiol	1.0E4-1.8E4 (2.6E1-4.4E1)		4.9E4** (8.5E1)**					
Methane	2.1E7-3.1E7	3.2E7	4.0E7***	--	1.1E7	2.0E7	7.5E6	6.7E7-8.4E7
Ammonia	4.9E4-1.3E5 (1.2E2-4.0E2)	3.3E6 (1.6E4)	--	4.2E6 (5.5E3)	--	--	--	--
Toluene	3.9E5-6.9E5 (9.4E2-1.7E3)	--	--	--	--	--	--	--
Xylenes	1.3E5-2.5E5 (3.4E2-6.2E2)	--	--	--	--	--	--	--

†Production factors in parenthesis.
--Blanks in table indicate values not available.
*Includes carbon disulfide.
**Includes other thiols.
***Includes C_2H_4.

TABLE 18. COMPARISON OF CONCENTRATION OF SIGNIFICANT PRODUCT GAS CONSTITUENTS WITH COMBUSTION FLUE GAS AND PARTICULATES, AMBIENT BACKGROUND CONCENTRATION, AND NIOSH-RECCMMENDED EXPOSURE LIMIT

	Fluidized-Bed[36] Coal Combustion [Flue Gas from Particulates]	Air Polluted[37] By Coal Tar Pitch [Analyzed from Particulates]	Residential[37] Coal Furnace Particulate Effluents	Ambient Air[30] Urban Average	Ambient Air[30] Nonurban Average	Permissible[39] Exposure Limit NIOSH Recommended Standard	Atmospheric[40] Organic Aerosol (Average)	Mean (This Study)
Carbon Monoxide	6.2E4			∿1.1E3⁺		4.0E4		2.3E8
Benzene				∿2.1E1⁺	∿2.1E0⁺			2.1E6
Hydrogen Sulfide						1.5E4		4.5E6
Carbon Dioxide	2.4E7					9.0E6**		2.3E8
Methanethiol						2.0E4**		1.4E4
Carbon Disulfide						3.0E3		1.9E4
Cresols							4.1E-2	6.2E4
Phenols							5.1E-2	1.1E5
Ammonia	5.0E2					3.5E4		8.8E4
Hydrogen Cyanide	1.2E0							2.2E4
Naphthalene							5.0E-2	1.2E5
Toluene				∿4.5E1⁺	∿4.5E0⁺			5.2E5
Diphenylmethane							2.6E-2	1.3E3
Phenanthrene	5.3E-3*	4.0E0	1.8E3				9.5E-3	8.8E2
Xylenes				∿2.8E1⁺	∿2.8E0⁺		4.9E-1	4.4E5
Benzo(a)pyrene	5.0E-4	4.0E-1	1.0E3	1.4E-2	1.7E-3			
Anthracene		8.0E-1	7.8E2	9.9E-4				9.8E2
Perylene		5.0E-2	1.2E2	2.8E-3			1.8E-2	
Pyrene	9.0E-3	8.3E0	2.2E3	1.4E-2			4.0E-2	4.7E0

*Includes anthracene.

⁺Private communication, William Lonneman, EPA

**Federal Occupational Standard.

be of major environmental concern (mean DS exceeds 50), as seen in Table 11. Examination of Table 15 shows that, based on MEG methodology, the aqueous condensate stream is the most hazardous effluent stream from the RTI gasifier, with a stream discharge severity of 2×10^5. About 96 percent of the overall discharge severity of this stream is contributed by cresols and xylenols. As mentioned before, the DMEG of phenol was recently increased thereby making it less severe. At this writing, DMEGs for cresols and xylenols were also being revised. Such an increase, if similar in magnitude to the increase in the phenol DMEG, would result in a considerable lowering of the overall discharge severity of the aqueous condensate effluent stream and would make ammonia, sulfides, arsenic, thiocyanates, and benzo(a)pyrene the most hazardous components in this stream.

Ranges of concentrations, production factors, and control priorities of significant aqueous condensate constituents may be seen in Figures 10, 14, and 18. A maximum variation of about four orders of magnitude is seen for the individual constituents. Considering the 95 percent confidence interval around the arithmetic mean as the most probable range, the maximum variation reduces to two orders of magnitude for all compounds with a variation of one order of magnitude or less for the most significant constituents (DS > 50), except sulfides. Sulfides show a greater variation because of the wide range of sulfur content of the coals gasified.

A comparison of the production factor and concentrations of significant constituents of the RTI gasifier aqueous condensate with those in the aqueous effluents of other gasifiers is presented in Table 19. The 95 percent confidence interval compares quite favorably to values for larger scale gasifiers, generally being within an order of magnitude of these values. Differences may be attributed to differences in analytical techniques or differences in processes.

This agreement may be seen more dramatically in Figure 25, which compares the concentrations of significant constituents of an aqueous condensate from the RTI gasifier with concentrations in the aqueous condensate from the Synthane gasifier, both from the gasification of Illinois No.6 coal. This agreement supports the ability of the RTI bench-scale unit in its ability to simulate larger gasifiers with respect to pollutant production. Arsenic levels are somewhat higher in the RTI gasifier than in other gasifiers. This may be due to differences in the process which result in a more efficient removal of arsenic from the gas stream by the condensation system for the RTI gasifier or to the general uncertainty associated with all trace element analysis. In summary, RTI condensate pollutant levels are remarkably similar to those of other gasifiers, especially considering differences in condensation or quench temperatures and procedures which exist in other gasification processes.

Comparison of pollutant levels in the RTI gasifier condensate with pollutant levels in the aqueous effluents from other coal conversion processes, ambient levels in U.S. waters, and regulated levels are given in Table 20. Comparisons with most stringent effluent standards for the United States and Canada and with end-of-pipe effluent standards set by the State of Illinois, suggest that in certain locations, aqueous effluents will have

TABLE 19. COMPARISON OF CONCENTRATION [μg/L] AND PRODUCTION FACTORS[+] [μg/g coal] OF SIGNIFICANT AQUEOUS CONDENSATE CONSTITUENTS FROM DIFFERENT GASIFIERS

Aqueous Condensate Pollutants (RTI Ranking)	RTI 95% Confidence μg/L (μg/g coal)	Chapman Gasifier[27] (Virginia Bituminous Coal)	Texaco Gasifier[44]		Lurgi Gasifier Separator Liuuor[45]		DOE/GFETC Condensate[30] North Dakota Lignite
			Illinois No.6	Western Coal	Illinois No.6	Montana Rosebud	
Cresols	4.8E5-8.8E5 (2.4E2-4.4E2)						2.0E6 (4.0E2)
Xylenols	1.4E4-3.2E5 (5.7E1-1.8E2)						4.5E5 (9.1E1)
Ammonia	4.8E6-7.8E6 (2.4E3-3.8E3)	5.0E6	1.3E6	2.7E6	1.7E6 (3.6E3)	4.0E6 (3.7E3)	8.4E6 (2.3E3)
Sulfides	0.0E0-4.7E5 (0.0E0-2.0E2)	<1.0E4	3.2E5	6.1E4	2.5E4 (5.2E1)	1.3E5 (1.2E2)	2.1E5 (5.8E1)
Arsenic	1.6E2-1.2E3 (2.3E-1-1.2E0)	8.0E2	2.2E1	1.6E1		1.4E1 (1.3E-2)	
Thiocyanates	1.5E5-3.1E5 (6.5E1-2.3E2)	7.0E1	8.0E3	2.9E4	6.5E4 (1.4E2)	6.0E3 (5.6E0)	
Phenol	7.9E5-1.6E6 (3.6E2-7.2E2)	3.0E5	<1.0E1	1.2E0	2.2E6 (4.6E3)	4.2E6 (3.9E3)	5.6E6 (1.1E3)
Cadmium	0.0E0-2.1E2 (0.0E0-2.5E-1)	5.0E0	3.0E0	<1.0E0		1.0E2 (9.3E-2)	
Selenium	2.5E2-1.0E3 (1.3E-1-4.9E-1)	2.0E3	1.0E1	4.6E2		5.0E1 (4.6E-2)	
Chromium	3.6E2-3.0E3 (4.2E-1-2.8E0)		6.0E0	<1.0E0		1.3E3 (1.2E0)	
Cyanide	1.5E3-7.3E3 (8.3E-1-4.4E0)	1.0E6	8.0E3	1.1E4	3.0E3 (6.3E0)	2.0E3 (1.9E0)	
Iron	4.7E3-5.1E3 (4.6E-1-6.7E0)	1.0E3					
Chlorides	9.4E5-2.7E6 (4.4E2-1.4E3)	3.0E6	7.4E5	7.5E3			
Silver	0.0E0-1.5E2 (0.4.1E-2)	2.0E0	2.0E0	<2.0E0		1.7E1 (1.6E-2)	
Lead	1.1E1-2.9E2 (3.3E-2-1.4E-1)		5.4E1	<5.0E0		1.2E2 (1.1E-1)	

[+] Production factors in parentheses.

continued

TABLE 19 (continued).

Aqueous Condensate Pollutants (RTI Ranking)	RTI 95% Confidence µg/L (µg/g coal)	Synthane PDU Gasifier Condensate Oxygen-Blown[41,42,43]				Air-Blown[33]	
		Illinois No.6	North Dakota Lignite	Wyoming Subbituminous	Illinois No.6 (3 Tests)	Illinois No.6	Montana Rosebud
Cresols	4.8E5-8.8E5 (2.4E2-4.4E2)	2.7E6 (2.5E3)	1.7E6 (8.5E2)	2.1E6 (1.0E3)			
Xylenols	1.4E5-3.2E5 (5.7E1-1.8E2)	9.4E5 (8.7E2)	4.5E5 (2.3E2)	4.5E5 (2.2E2)			
Ammonia	4.8E6-7.8E6 (2.4E3-3.8E3)	8.1E6 (7.5E3)	7.2E6 (3.6E3)	9.5E6 (4.8E3)		5.9E6 (1.7E3)	2.6E7 (1.3E4)
Sulfides	0.0E0-4.7E5 (0.0E0-2.0E2)						
Arsenic	1.6E2-1.2E3 (2.3E-1-1.2E0)	3.6E1 (3.3E-2)			1.0E0 (1.4E-3)		
Thiocyanates	1.5E5-3.1E5 (6.5E1-2.3E2)	1.5E5 (1.4E2)	2.2E4 (1.1E1)	2.3E4 (1.1E1)		2.4E5 (6.9E1)	4.3E4 (2.2E1)
Phenol	7.9E5-1.6E6 (3.6E2-7.2E2)	2.6E6 (2.4E3)	2.8E6 (1.4E3)	4.1E6 (2.0E3)		2.8E6 (8.0E2)	2.5E6 (1.3E3)
Cadmium	0.0E0-2.1E2 (0.0E0-2.5E-1)						
Selenium	2.5E2-1.0E3 (1.3E-1-4.9E-1)	3.6E2 (3.3E-1)			1.1E2 (1.5E-1)		
Chromium	3.6E2-3.0E3 (4.2E-1-2.8E0)	6.0E0 (5.5E-3)			1.8E1 (2.5E-2)		
Cyanide	1.5E3-7.3E3 (8.3E-1-4.4E0)	6.0E2 (5.5E-1)	1.0E2 (5.0E-2)	2.3E2 (1.1E-1)		2.0E3 (5.7E-1)	1.0E3 (5.1E-1)
Iron	4.7E3-5.1E3 (4.6E-1-6.7E0)	2.7E3 (2.5E0)			1.2E2 (1.7E-1)		
Chlorides	9.4E5-2.7E6 (4.4E2-1.4E3)	5.0E5 (4.5E2)				2.4E5 (6.9E1)	6.3E4 (3.2E1)
Silver	0.0E0-1.5E2 (0-4.1E-2)						
Lead	1.1E1-2.9E2 (3.3E-2-1.4E-1)				2.5E0 (3.5E-3)		

continued

+Production factors in parentheses.

TABLE 19 (continued).

Aqueous Condensate Pollutants (RTI Ranking)	RTI 95% Confidence μg/L (μg/g coal)	Hygas Gasifier Condensate[46] Montana Subbituminous	Hygas Gasifier Condensate[46] Illinois No.6	CO_2-Acceptor Gas Quench Water Blowdown North Dakota Lignite[34]	COED Pilot Plant Scrubber Liquor First Stage	COED Pilot Plant Scrubber Liquor Second Stage	Koppers Totzek[48] Gasifier Aqueous Effluent
Cresols	4.8E5-8.3E5 (2.4E2-4.4E2)						
Xylenols	1.4E5-3.2E5 (5.7E1-1.8E2)						
Ammonia	4.8E6-7.8E6 (2.4E3-3.8E3)	6.0E6 (6.6E3)	6.5E6	1.3E6 (1.0E4)			1.4E5
Sulfides	0.0E0-4.7E5 (0.0E0-2.0E2)	1.9E5 (2.1E2)	1.1E6	2.8E4 (2.2E2)			
Arsenic	1.6E2-1.2E3 (2.3E-1-1.2E0)				1.0E1	7.0E2	
Thiocyanates	1.5E5-3.1E5 (6.5E1-2.3E2)	2.1E5 (2.3E2)	1.0E5				
Phenol	7.9E5-1.6E6 (3.6E2-7.2E2)	4.4E6 (4.8E3)	1.2E6	1.8E1 (1.4E-1)			
Cadmium	0.0E0-2.1E2 (0.0E0-2.5E-1)				<3.0E2	<3.0E2	
Selenium	2.5E2-1.0E3 (1.3E-1-4.9E-1)						
Chromium	3.6E2-3.0E3 (4.2E-1-2.8E0)				1.0E3	1.0E3	
Cyanide	1.5E3-7.3E3 (8.3E-1-4.4E0)	1.0E1 (1.1E-2)	<1.0E0	2.0E1 (1.6E-1)			1.4E3
Iron	4.7E3-5.1E3 (4.6E-1-6.7E0)		2.3E6	7.3E1 (5.8E-1)	3.0E5	5.0E5	2.0E2
Chlorides	9.4E5-2.7E6 (4.4E2-1.4E3)		6.5E3	5.6E4 (4.5E2)			5.7E4
Silver	0.0E0-1.5E2 (0-4.1E-2)		<2.5E4				
Lead	1.1E1-2.9E2 (3.3E-2-1.4E-1)		<6.0E4		1.0E2	2.0E3	

+Production factors in parenetheses.

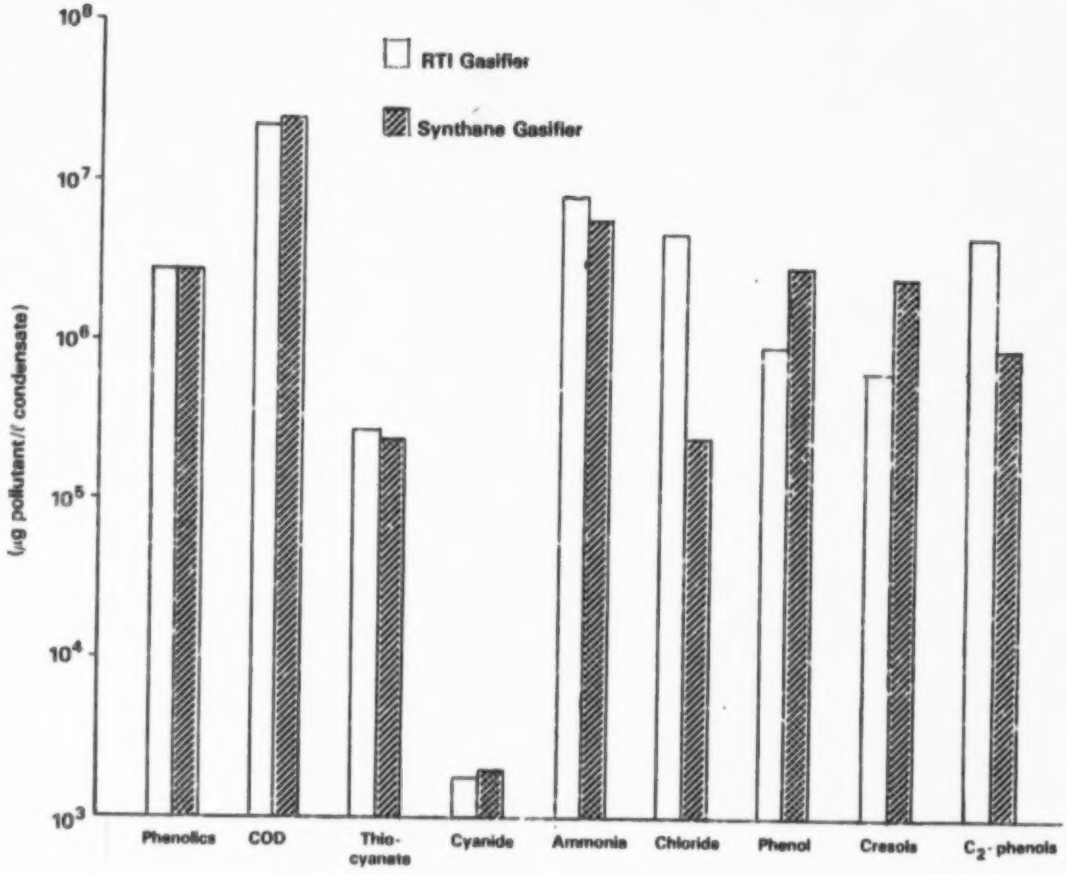

Figure 25. Aqueous condensate pollutant production from gasification of Illinois No.6 coal.

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TABLE 20. COMPARISONS OF CONCENTRATIONS [μg/L] OF SIGNIFICANT AQUEOUS CONDENSATE CONSTITUENTS WITH CONCENTRATIONS IN EFFLUENTS FROM OTHER COAL CONVERSION PROCESSES, AMBIENT LEVELS, AND REGULATED LEVELS

	RTI 95% C.I.	Coke Plant[49] Waste Ammonia Liquor Range	Coal Ash[50] Pond Effluent	Coke Plant[51] Liquor	SRC-I[51] Wastewater	H-Coal Foul[52] Process Water	SRC[53] Wastewater
Cresols	4.8E5-8.8E5						9.4E5
Xylenols	1.4E5-3.2E5						3.8E5
Ammonia	4.8E6-7.8E6	1.8E6-4.3E6	5.0E1	5.0E6	5.6E6		
Sulfides	0-4.7E5	0-5.0E4		1.3E6	4.0E6		
Arsenic	1.6E2-1.2E3		2.0E1				
Thiocyanates	1.5E5-3.1E5	1.0E5-1.5E6		1.0E6			
Phenol	7.9E5-1.6E6	4.1E5-2.4E6	<2.5E1	1.6E6	4.5E6		3.9E5
Cadmium	0-2.1E2		<1.0E2			8.0E2	
Selenium	2.5E2-1.0E3						8.0E2
Chromium	3.6E2-3.0E3					1.0E2	9.0E4
Cyanide	1.5E3-7.3E3	1.0E4-3.7E4	<1.0E1	5.0E4		1.0E4	
Iron	4.7E3-5.1E3		5.0E2			1.2E3	5.6E5
Chlorides	9.4E5-2.7E6			6.0E6			
Silver	0-1.5E2						
Lead	1.1E1-2.9E2		<5.0E1			2.9E3	

continued

TABLE 20 (continued).

	RTI 95% C.I.	Wabash[52] River Indiana	Fresh[54] Water	Rivers &[54] Lakes Mean of 8 Regions	Most Stringent[53] Water Quality Standards (U.S.)	Most Stringent[53] Effluent Limitations (U.S. & Canada)	EPA NIPDWS°	Illinois[53] Effluent Standards (all point sources)
Cresols	4.8E5-8.8E5							
Xylenols	1.4E5-3.2E5							
Ammonia	4.8E6-7.8E6	8.0E1			2.0E1	5.0E2		
Sulfides	0-4.7E5					1.1E1		
Arsenic	1.6E2-1.2E3	2.0E0	4.0E-4	8.1E1	1.0E1	5.0E1	5.0E1	2.5E2
Thiocyanates	1.5E5-3.1E5							
Phenol	7.9E5-1.6E6	1.0E0+			1.0E0+	5.0E0+		3.0E2
Cadmium	0-2.1E2	<1.0E0		1.2E1	2.0E0	5.0E0	1.0E1	1.5E2
Selenium	2.5E2-1.0E3	1.0E0	<2.0E-2		5.0E0	1.0E1	1.0E1	
Chromium	3.6E2-3.0E3	<1.0E1	1.8E-4		5.0E1	5.0E1*	5.0E1*	3.0E2*
Cyanide	1.5E3-7.3E3	0.0E0			5.0E0	2.0E1		2.5E1
Iron	4.7E3-5.1E3	1.8E3	6.7E-1	4.3E1	3.0E2	3.0E2		2.0E3
Chlorides	9.4E5-2.7E6	2.3E4	7.8E0		1.0E5	2.5E5		
Silver	0-1.5E2	0.0E0	1.3E-4	2.2E0	1.0E-1	5.0E1	5.0E1	1.0E2
Lead	1.1E1-2.9E2	4.0E1	2.2E1	2.2E1	1.0E2	5.0E1	5.0E1	1.0F2

*Hexavalent Cr
+Total Phenols
°National Interim Primary Drinking Water Standards

to be processed to reduce the levels of all the pollutants listed. Considering the variation in the chemical nature of these pollutants, a diverse approach may be necessary when deciding on wastewater treatment options, and several techniques will have to be combined for proper treatment in areas, such as Illinois, with strong regulations of effluent composition.

Comparison of the levels of the pollutants ammonia, sulfides, thiocyanates, phenol, and cyanides in the RTI condensate with coke plant liquors suggests that these streams are very similar in gross chemical composition. Point source effluent limitations have been established by the EPA for aqueous effluents from byproduct coking plants under the Clean Water Act.[55] Cyanide, phenol, ammonia, and sulfide are regulated under these source-based effluent limitations. As a result, control techniques have been developed for these streams and are presently well-established technology. Because of the similarity between coke plant liquor and gasifier condensate, this technology from the coking industry can probably be easily applied to gasifier aqueous condensate.

Similarly, point source effluent limitations also have been established for certain aqueous effluents from petroleum refining, and techniques developed for pollution control in these streams may also be applicable to gasification wastewater.[51] Thus, the basic technology for the control of major pollutants in gasifier wastewater streams is already available, although certain modifications may be necessary for the proper application of these technologies.

As mentioned before, PNAs were analyzed by GC^2 in the extract of one sample of aqueous condensate from the gasification of North Dakota lignite (test 43). The results of this analysis are presented in Table 21; but because this was a single analysis, any conclusions drawn from this analysis should be viewed with caution. Examination of Table 21 shows that several priority pollutants and several carcinogenic compounds may be found in gasifier condensate. Only benzo(a)pyrene had a concentration above the DMEG value, with a discharge severity of 120. However, increased emphasis which recent legislation has placed on carcinogenic substances may eventually result in regulations which require zero discharges of carcinogenic compounds. For zero discharge to be achieved, the only certain treatment presently available is forced evaporation followed by incineration of the remaining wastes, a process involving severe energy penalties, high capital cost, and possible emissions of toxic substances to the air.[56] It therefore may be necessary to develop advanced control techniques for these trace organics in coal conversion waters if zero discharge is to be achieved in an economical, energy-efficient manner.

6.4 TAR

Crude tar produced from the RTI laboratory coal gasifier was found to be extremely complex with a variety of organic acids, bases, polynuclear aromatics and other neutral compounds. A fractionation scheme[2] produced six fractions, ranges of which were shown in Figure 21. Details of GC^2 analysis of crude tar were presented in Section 3.2. Although over 70 tar constituents were quantitated in the various gasification tests and some 300 were

TABLE 21. PNA COMPOUNDS DETECTED IN THE AQUEOUS CONDENSATE FROM THE GASIFICATION OF NORTH DAKOTA LIGNITE (TEST 43)

Compound		Concentration	DMEG Water/Health
2-Methylnaphthalene	●	2.2E2	3.4E6
Anthracene	* ▲	4.1E1	8.4E5
Phenanthrene	* ▲	9.6E1	2.4E4
Acenaphthylene	▲ ●	5.7E1	
Chrysene	* ▲	1.6E2	3.3E4
Triphenylene		5.0E1	
Fluorene	▲ ●	5.7E1	
Fluoranthene	▲ ●	2.8E1	1.4E6
Benzo(a)pyrene	* ▲	3.6E1	3.0E-1
Benzo(e)pyrene	*	2.1E1	4.6E4
Perylene	●	2.1E1	
Benzo(k)fluoranthene	* ▲	1.7E1	2.4E4
Benzo(b)fluoranthene	* ▲	3.3E1	1.3E4

*Carcinogens.

▲Priority pollutants.
●Suspected carcinogens.

qualitatively identified, tar as such still remains obscure because of the presence of thousands of compounds. Fortunately, most of the important constituents were quantitated. Several constituents were eliminated from consideration based on MEG methodology. Nineteen constituents could not be eliminated based on their maximum concentration and were ranked according to discharge severity (Tables 8 and 12). Additionally, some of the sulfur heterocyclics (notably phenanthro(4,5-bcd)thiophene and heavier) could not be eliminated from consideration since they have recently been shown to be mutagenic[11] and no DMEG has yet been assigned to them. Among the 19 important constituents, the five most severe are cresols, xylenols, trimethylphenol, dibenzo(a,h)anthracene, and benzo(a)pyrene. More than 85 percent of the overall stream severity is contributed by cresols and xylenols. Recently, as stated earlier, the DMEG of phenol was increased making it less severe. This made it rank number 15 in the tar stream. At this writing, DMEGs for cresols and xylenols are being revised. Thus, presumably the most severe constituents are PAHs, namely, dibenzo(a,h)anthracene and benzo(a)pyrene. The bioassay results (Section 5.4) show both the PAHs and tar bases to be mutagenic in many cases. It is believed that most of the mutagenicity to tar bases is contributed by primary aromatic amines. These compounds are more likely to be present in tars formed at lower temperatures (e.g., from low temperature carbonization). The continuous run tars compared to the semibatch tar supports this view (see Section 5.4) for the RTI laboratory study. More research needs to be carried out in the evaluation of aromatic amines and sulfur heterocyclics in coal gasification tar. Analytical difficulties are the main cause of hindrance at present (see Section 2.4).

Concentration, production factor, and control priority ranges for significant tar constituents were presented in Figures 11, 15, and 19, respectively. A maximum variation of up to three orders of magnitude is seen with the 95 percent confidence limits around the mean being generally much less than one order of magnitude. Control technology for tar will depend on its ultimate fate. Some tar may be recirculated to the gasifier, some may be hydrotreated and hydrogenated, and some may be combusted. It appears that a proper control on the levels of the two most severe PAHs listed earlier should be the control criteria for any emissions causing contact with the crude tar itself.

A comparison of the production factor and concentrations for the RTI gasifier tars to other gasifiers is made in Table 22. A major conclusion from the table (although detailed tar analyses in literature are quite obscure) is that good agreement in production and composition exists between the RTI tars and those from larger processes. If a coal conversion process produces coal tar (some of the gasification processes such as those utilizing entrained beds do not produce any tar due to cocurrent flow and high temperature), then all compounds are very likely to appear in all tars; i.e., they should be qualitatively similar. Also, gross compositional differences do not exist, as seen from Table 22. The phenol content apparently is quite temperature-dependent even at lower heating rates and low overall temperatures. This observation has also been made by operating the RTI gasifier in a continuous mode as opposed to a batch mode. The major

TABLE 22. COMPARISON OF RTI TAR COMPOSITION AND PRODUCTION TO THOSE FROM OTHER GASIFIERS

	RTI Range 95% Confidence	Synthane[34] Illinois No.6	METC[55]	Chapman[27], Wilputte	GFETC[30,34]	Coal Tar	Coal Tar 2
Total Tar (mg/g coal)	15-23	37	26-34	100	12-36		
Cresols	1.1E4-2.3E4		1.8E4*			8.0E3	
Xylenols	7.1E3-1.7E4					2.0E3	
Dibenzo(a,h)anthracene	7.5E2-2.1E3						2.3E2
Benzo(a)pyrene	1.5E3-2.5E3		4.0E3	8.0E2	7.0E3[+]		1.8E3
Perylene	1.1E3-2.5E3			8.0E2			8.0E3
Benzo(a)anthracene	2.6E3-5.6E3						7.0E3
Benzo(g,h,i)perylene	3.6E2-1.6E3						1.9E3
Phenanthrene	1.9E4-4.1E4	1.2E5**			4.2E4	5.0E4	1.8E4
Naphthalene	3.7E4-1.1E5	7.0E4	2.1E4	2.0E3	6.3E4	1.0E5	
Acenaphthylene	1.5E4-2.9E4					2.0E4	
Pyrene	8.2E3-2.4E4	4.2E4			2.5E4	2.1E4	1.1E4
Phenol	4.5E3-1.1E4	1.2E4	4.0E2	2.0E3	1.0E5	4.0E3	
Biphenyl	2.6E3-4.0E3				1.6E4	4.0E3	
Acenaphthene	3.2E3-5.6E3	1.2E5*				3.0E3	
Chrysene	2.8E3-5.6E3	7.6E4**		3.0E3	1.4E4	2.0E4	2.9E4

*Analysis of pollutant class.

**Includes anthracene.

***Includes benzo(a)anthracene.

[+] Includes benzo(e)pyrene.

elemental compositions of tars from different tar-producing gasifiers are similar (Table 23) also.

A comparison of significant coal gasifier tar constituents to coal liquefaction products, petroleum asphalt, shale oil naphtha and combustion, and incinerator particulates is shown in Table 24. Striking features of the table are that (a) coal liquids and gasifier tars contain similar compounds although presumably the boiling point distribution (and quantitative composition) may be quite different, (b) shale oil naphtha contains PCX at only about one order of magnitude lower level than gasifier tars, (c) combustion of coal produces particulates resulting in a far lower order of magnitude of PAHs, and (d) petroleum asphalt contains PAHs at near background (i.e., many orders of magnitude lower) concentrations whereas coal tar pitch contains larger amounts of heavy PAHs. Aminonaphthalenes in SRC-II distillate shown to be mutagenic by Felix et al.[12] are quite close in levels to RTI gasifier tar whose base fractions have in various cases been shown to be mutagenic (see Section 6.4).

In conclusion, tars are complex and hazardous but do not represent as much of a containment problem (primarily because of a lot smaller volume) as the condensate. The tar stream can be isolated from the water using conventional coke plant technology. Three methods of utilization include recycle to gasifier, combustion, hydrotreating to valuable chemical stock or possibly a combination of these.

6.5 ASH

RTI gasifier ash was analyzed for trace elements by AA and NAA. Details of the analytical techniques employed are available elsewhere.[2,70] Out of some 26 elements analyzed, only nine trace elements exceeded their DMEG (land/health) in the gasifier ash. None of these elements have a mean discharge severity over 50 and only two elements, arsenic and chromium, have a discharge severity over 25. Ranges of concentrations, production factors, and control priorities are shown in Figures 12, 15, and 20, respectively. A maximum variation of about three orders of magnitude is seen in these figures. Considering the 95 percent confidence interval around the arithmetic mean, the maximum variation reduces to one order of magnitude for the concentrations of all significant ash constituents.

Table 25 shows a comparison of the RTI gasifier ash trace element concentrations to those for other larger scale gasifiers. Trace element concentrations in the ashes from larger scale gasifiers are generally within an order of magnitude of the concentration range for the RTI gasifier ash. This agreement is very good considering the range of potential variation of trace element concentrations in U.S. coals and the problems inherent in any trace metal analysis including sampling of representative material and matrix effects.

Table 26 is a comparison of RTI gasifier ash trace metal concentrations with concentrations in combustion ashes, raw coal, and a typical shale. Most of the elements in this table have similar concentrations in combustion

TABLE 23. TAR COMPOSITION FOR VARIOUS PROCESSES (%)

Process	Coal	Carbon	Hydrogen	Nitrogen	Sulfur	Oxygen
Lurgi[34]	Montana Rosebud Subbituminous A	83.1*	7.7	0.7	0.3	8.2
	Illinois No.6	85.5	6.4	1.2	1.7	5.2
	Illinois No.5	85.9	6.4	1.2	2.4	4.2
	Pittsburgh No.8	88.5	5.9	0.9	1.5	3.2
Slagging GFETC[34]	Indian Head North Dakota Lignite	83.7	8.7	0.9	0.5	5.9
Synthane (Air-Blown)[33]	Illinois No.6	82.7	6.4	1.3	2.5	7.1
	North Dakota Lignite	86.7	6.5	1.2	0.8	5.1
	Montana Subbituminous	87.5	6.4	1.2	0.6	4.3
Chapman-Wilputte[27]	Virginia Bituminous	77.3	6.1	1.4	0.5	NA
RTI Laboratory Gasifier	Illinois No.6 Batch (Average of 5)	86.2	6.3	1.4	1.9	4.1
	Western Kentucky No.9 Batch	86.3	6.1	1.6	2.7	2.9
	Wyoming Subbituminous Batch (Average of 3)	83.5	7.2	1.1	1.5	6.5
	North Dakota Lignite Batch (Average of 4)	82.8	7.2	1.3	1.3	6.8
Average of All Processes and Coals		84.8	6.7	1.1	1.4	4.8

TABLE 24 (continued).

	Mean (This Study)	Shale Oil[65] Naphtha	Petroleum[66] Asphalt	Coal Tar Pitch[66]	Synthoil[67]	Commercial Incinerator Particulates[68] (Multiple Chamber)
Cresols	1.7E4(3.4E2)	8.8E3				
Xylenols	1.2E4(2.4E2)	2.8E3				
Dibenzo(a,h)anthracene	1.4E391.9E1)					
Benzo(a)pyrene	2.5E3(3.3E1)		5.0E-1	1.0E4	4.1E1	1.8E2
Perylene	1.8E3(2.3E1)		<5.0E-1	2.7E3		3.6E1
Benzo(a)anthracene	4.1E3(5.6E1)		1.5E-1	1.1E4	1.8E1	
Benzo(g,h,i)perylene	1.0E3(1.2E1)		2.1E0	3.2E3		5.4E2
Phenanthrene	3.0E4(3.8E2)		2.3E0	3.0E4	4.1E2	6.2E1
Arsenic	2.1E0⁺(5.4E-2)					
Naphthalene	7.1E4(3.2E2)					
Acenaphthylene	2.2E4(2.6E2)				2.0E1	
Pyrene	1.6E4(1.6E2)		6.0E-1	2.5E4		2.6E3
Phenol	7.7E3(1.6E2)	1.6E3				
Biphenyl	3.3E3(5.1E1)				8.9E1	
Acenaphthene	4.4E3(9.9E1)				6.1E1	
Chromium	3.6E1⁺(1.5E0)*					
Chrysene	4.2E3(6.0E1)		2.0E-1	8.7E3	9.8E1	
Aminonaphthalenes	1.0E2(2.1E0)					

Production factors (μg/g coal) in parentheses.

⁺Mean value for As = 1.4E1 and Cr = 1.4E1 for 101 coals (Reference 64).

*High chromium value is likely due to the stainless steel reactor.

continued

TABLE 24. COMPARISON OF CONCENTRATIONS [µg/g] OF COAL GASIFICATION TAR CONSTITUENTS WITH COAL LIQUIDS, ASPHALT, PITCH AND COMBUSTION PARTICULATES

	Mean (This Study)	SRC-II[12] Distillate	SRC-I[61] Extract	SRC Light[62] Oil	Low Temperature[63] Carbonization		COED[59]	
					500°C	650°C	Raw Oil	Syncrude
Cresols	1.7E4(3.4E2)	4.1E4			1.1E4	1.6E4		
Xylenols	1.2E4(2.4E2)	3.5E4			6.6E4			
Dibenzo(a,h)anthracene)	1.4E3(1.9E1)		2.3E2					
Benzo(a)pyrene	2.5E3(3.3E1)	4.1E1	7.1E2				1.1E2	5.1E1
Perylene	1.8E3(2.3E1)		1.9E2					
Benzo(a)anthracene	4.1E3(5.6E1)		5.0E2				4.2E1	Trace
Benzo(g,h,i)perylene	1.0E3(1.2E1)							
Phenanthrene	3.0E4(3.8E2)		5.7E3	2.5E1				
Arsenic	2.1E0[+](5.4E-2)						3.0E0[+]	2.0E0[+]
Naphthalene	7.1E4(3.2E2)	9.7E4		1.6E3	6.0E2	1.0E4		
Acenaphthylene	2.2E4(2.6E2)			2.0E0				
Pyrene	1.6E4(1.6E2)		6.7E3	2.0E1	3.1E3	1.5E4	2.7E2	Trace
Phenol	7.7E3(1.6E2)	2.7E4						
Biphenyl	3.3E3(5.1E1)	2.4E4	2.1E1	8.0E1	2.9E3	1.1E4		
Acenaphthene	4.4E3(9.9E1)							
Chromium	3.6E1[+](1.5E0)*						2.0E0[+]	7.0E-1[+]
Chrysene	4.2E3(6.0E1)		2.0E3					
Aminonaphthalenes	1.0E2(2.1E0)	9.0E1						

Production factors (µg/g coal) in parentheses.

[+] Mean value for As ≡ 1.4E1 and Cr ≡ 1.4E1 for 101 coals (Reference 64).

[*] High chromium value is very likely due to the stainless steel reactor used.

TABLE 24 (continued).

	Mean (This Study)	Opening Burning Municipal Refuse Incineration Smoke Plume[68]	Pulverized Coal Combustion[69]			
			Vertically-Fired Dry Bottom	Front Wall-Fired Dry Bottom	Tangentially-Fired Dry Bottom	Cyclone-Fired Wet Bottom
Cresols	1.7E4(3.4E2)					
Xylenols	1.2E4(2.4E2)					
Dibenzo(a,h)anthracene	1.4E3(1.9E1)	1.1E1	(3.8E-3)	(6.0E-4)	(4.6E-3)	(1.9E-2)
Benzo(a)pyrene	2.5E3(3.3E1)		(7.0E-4)		(2.3E-3)	(1.8E-3)
Perylene	1.8E3(2.3E1)					
Benzo(a)anthracene	4.1E3(5.6E1)					
Benzo(g,h,i)perylene	1.0E3(1.2E1)		(2.4E-3)	(5.0E-4)	(4.9E-3)	(1.7E-3)
Phenanthrene	3.0E4(3.8E2)			(7.3E-3)	(1.1E-3)	
Arsenic	2.1E0⁺(5.4E-2)					
Naphthalene	7.1E4(3.2E2)					
Acenaphthylene	2.2E4(2.6E2)					
Pyrene	1.6E4(1.6E2)	2.9E1	(2.1E-3)	(7.3E-3)	(4.6E-3)	(8.6E-2)
Phenol	7.3E3(1.6E2)					
Biphenyl	3.3E3(5.1E1)					
Acenaphthene	4.4E3(9.9E1)					
Chromium	3.6E1⁺(1.5E0)*					
Chrysene	4.2E3(6.0E1)					
Aminonaphthalenes	1.0E2(2.1E0)					

Production factors (μg/g coal) in parentheses.

⁺Mean value for As = 1.4E1 and Cr = 1.4E1 for 101 coals (Reference 64).

*High chromium value is very likely due to the stainless steel reactor used.

TABLE 25. COMPARISONS OF CONCENTRATIONS [µg/g] OF SIGNIFICANT ASH CONSTITUENTS FROM DIFFERENT GASIFIERS

	RTI Gasifier Ash (95% Confidence Interval)	Synthane[71] Gasifier Ash		Chapman[27] Gasifier Ash	Lurgi Gasifier Ash[72]			Texaco Gasifier[44] Slag	
		Montana Rosebud	Illinois No.6	Virginia Bituminous	North Dakota Lignite	Montana Rosebud	Illinois No.6	Illinois No.6	Western
Arsenic	1.2E1-2.4E1	7.6E0	4.2E0	<4.0E-1	7.4E1	2.6E1	1.0E-1	1.5E1	3.0E1
Chromium	8.2E2-2.4E3	2.4E1	1.9E2	3.0E1	1.4E2	4.4E2	7.5E2	1.8E3	2.1E3
Nickel	0-7.9E2	1.2E1	2.5E1		2.5E1	2.0E2	4.6E2	2.3E2	3.9E2
Manganese	1.9E2-3.5E2	2.0E3	3.0E2		7.6E2	7.9E2	2.0E2	6.1E2	3.8E2
Iron	3.9E4-1.0E5	1.3E4	>1.0E4	1.0E4	7.9E4	1.1E4	1.7E4		
Beryllium	3.9E0-1.1E1	5.3E0	4.1E0	1.0E0	6.0E0	2.8E0	1.4E1	7.5E0	2.2E0
Aluminum	5.2E4-7.6E4	3.8E4	1.9E3	3.0E3	6.3E4	1.8E1	2.0E4		
Sodium	1.3E4-6.3E4	1.8E3	>1.0E4		5.9E4				
Selenium	2.5E0-5.5E0	1.4E-1	4.4E0	3.0E1	5.0E-1	2.2E0		1.4E1	7.6E-1

TABLE 25 (continued).

	RTI Gasifier Ash (95% Confidence Interval)	Wellman-Galusha[28,73] Gasifier Ash		Hygas[74] Ash Pittsburgh No.8	COED[34] Process Char	CO_2-Acceptor[34] Gasifier Ash North Dakota Lignite
		Anthracite	North Dakota Lignite			
Arsenic	1.2E1-2.4E1	3.0E3	3.0E1	3.4E0	1.0E1	1.9E1
Chromium	8.2E2-2.4E3	1.9E2	2.1E1	1.5E1	3.0E2	3.0E1
Nickel	0-7.9E2	6.2E1	6.7E1	9.1E0	4.0E1	2.0E1
Manganese	1.9E2-3.5E2	6.9E1	6.4E1		1.0E2	
Iron	3.9E4-1.0E5	>1.0E3	3.0E4		2.0E4	
Beryllium	3.9E0-1.1E1	1.0E0	9.0E0	7.5E-1		5.0E0
Aluminum	5.2E4-7.6E4	>1.0E3	1.9E4		1.0E4	
Sodium	1.3E4-6.3E4	1.0E3	3.3E4		<5.0E2	
Selenium	2.5E0-5.5E0	2.0E0	1.5E1	4.4E-1	3.0E0	4.0E0

TABLE 26. COMPARISONS OF CONCENTRATIONS [μg/g] OF SIGNIFICANT TRACE ELEMENTS IN RTI GASIFIER ASH WITH COMBUSTION ASH, COAL, AND A TYPICAL SHALE

	RTI Gasifier Ash (95% C.I.*)	Combustion Bottom Ash[75]	Combustion[76] Bottom Ash (slag)	Combustion[76] Fly Ash	Mean (Geometric) - U.S. Coals[77]			Shale[54] (rock)
			Ill. Basin Coal		Eastern	Western	Ill. Basin	
Arsenic	1.2E1-2.4E1	8.0E-1	1.8E1	1.1E2	1.5E1	1.5E0	7.4E0	1.3E1
Chromium	8.2E2-2.4E3	6.0E2	1.5E2	3.0E2	1.8E1	8.1E0	1.6E1	9.0E1
Nickel	0-7.9E2		8.5E1	2.1E2	1.4E1	4.4E0	1.9E1	6.8E1
Manganese	1.9E2-3.5E2		2.9E2	3.0E2	1.2E1	2.8E1	4.0E1	8.5E3
Iron	3.9E4-1.0E5		1.1E5	1.2E5	1.3E4	4.9E3	1.9E4	<1.7E4
Beryllium	3.9E0-1.1E1	4.2E0			1.1E0	3.5E-1	1.6E0	3.0E0
Aluminum	5.2E4-7.6E4		1.0E5	9.1E4	1.6E4	8.8E3	1.2E4	
Sodium	1.3E4-6.3E4		5.0E3	1.0E4	3.0E2	6.0E2	3.0E-2	9.6E3
Selenium	2.5E0-5.5E0	2.6E0	8.0E-2	2.5E1	3.4E0	1.3E0	2.0E0	6.0E-1

*C.I. = Confidence Interval

bottom ash and gasifier ash. Chromium is higher in the RTI gasifier ash than in the combustion bottom ash because of the erosion of the stainless steel reactor in the RTI gasifier under the severe conditions of gasification. Sodium is also found in higher concentrations in the RTI gasifier ash. This could be because the conditions of gasification are less severe than combustion (i.e., lower temperatures), resulting in a greater retention of sodium in the ash, or this difference could reflect a difference in sodium concentrations in the feed coals to the processes. Differences in selenium concentrations in combustion and gasifier ash could be attributed to the same factors. Flyash is also similar to gasifier ash except for chromium, due to chromium enrichment in the gasifier ash, and for arsenic and selenium, which are probably higher in the flyash because of condensation of volatile arsenic and selenium onto flyash particles in the flue gas as it cools.

The U.S. Environmental Protection Agency has promulgated final regulations (40 CFR Part 261) on the identification and listing of hazardous wastes as required under the Resource Conservation and Recovery Act (RCRA) of 1976.[78] As stipulated by RCRA, these regulations include an extraction procedure (EP) to evaluate the leachability of toxic materials from solid wastes. Such a test is judged to provide a meaningful environmental evaluation of the potential groundwater contamination which could result from the improper disposal of the solid wastes in question. If the solid waste is deemed hazardous by the definition, it must be handled and disposed of according to rules set down in 40 CFR Parts 263, 264, and 265. Thus, EP enables potential problems with solid disposal to be anticipated and avoided.

The major solid waste from gasification processes is the reactor bottom ash or slag. The proper disposal of this waste is an important portion of the environmental protection required for any scaled-up versions of gasification processes. In order to define the status of these wastes as hazardous or nonhazardous, representative samples need to be subjected to the RCRA extraction procedure. This involves a batch leaching test using water acidified to a pH of 5 with acetic acid. A detailed description of the standard EP may be found in the Federal Register of May 19, 1980.[79] The extract from the EP is analyzed for eight elements (arsenic, barium, cadmium, chromium, lead, mercury, selenium, and silver) and other toxic chemicals specified in the EP. If the concentration of any of the eight elements in the extract exceeds 100 times the National Interim Primary Drinking Water Standards (NIPDWS) for these elements (Table 27), the waste is to be listed as hazardous and identified by the hazardous waste number corresponding to that element (Table 27). The factor of 100 was chosen to account for attenuation of the leachate concentration as it percolates down to groundwater level. If the waste is determined as hazardous using the EP, then it must be cared for in a "cradle to grave" manner as specified under RCRA.[79]

Although RTI gasifier ash has not been subjected to the EP, a few ashes from pilot and commercial-scale gasifiers have been tested for potential hazardous nature using the EP. None of seven gasification wastes tested were found to be hazardous under RCRA.[80,81,82] The concentrations of the eight elements of concern, in the extracts of these wastes, were two to five orders of magnitude below the maximum concentrations specified under RCRA for the

TABLE 27. MAXIMUM CONCENTRATIONS OF CONTAMINANTS FOR CHARACTERISTIC EP TOXICITY

EPA Hazardous Waste No.	Contaminant	Maximum Concentration (mg/L)
D004	Arsenic	5.0
D005	Barium	100.0
D006	Cadmium	1.0
D007	Chromium	5.0
D008	Lead	5.0
D009	Mercury	0.2
D010	Selenium	1.0
D011	Silver	5.0

waste to be considered hazardous (Table 27). These limited tests suggest that gasifier waste will be excluded from the RCRA requirements for handling, storing, and disposal of hazardous solid wastes, although ashes from the gasification of certain coals with exceptionally high concentrations of toxic elements could conceivably prove hazardous under RCRA. However, the extreme low levels of these elements reported for the EP extracts of gasification make this an outside possibility. For instance, worst case predictions for Lurgi gasifier residue from the gasification of coal with 120 ppm of arsenic (the maximum amount found in a U.S. coal) give a predicted value of 470 µg/L for the arsenic content of the EP extract, still an order of magnitude under the RCRA standard for arsenic of 5000 µg/L.[81] By predicting leachate concentration using the maximum reported concentrations of trace elements in U.S. coals and limited data from actual leaching tests, Yu and Crawford found that the only elements likely to be present in the EP extract above 100 x NIPDWS concentration were selenium in Texaco gasifier slag and cadmium in Lurgi ash and Texaco slag.[81] Coals with such high cadmium or selenium concentrations are very rare, and therefore most gasifier ash probably will prove nonhazardous under RCRA. Thus, ash from the RTI tests, using coals with more moderate trace element concentrations, would most likely also prove to be nonhazardous under RCRA guidelines.

Although gasifier ash appears nonhazardous under RCRA and does not require the extreme caution specified under RCRA for handling and storage, studies suggest that potential environmental problems may still exist for the landfill disposal of gasifier ash. Column leaching studies, undertaken to simulate more closely the natural movement of soluble constituents in a landfill, showed a high concentration pulse of certain elements in the leachate during the initial leaching period.[82,83] Similar pulses of certain trace metal concentrations have been noted during groundwater monitoring around a flyash disposal shortly after a rapid increase of the amount of flyash deposited in the pond.[84] Such short-term perturbations could conceivably create momentary high concentrations of elements entering the groundwater or nearby lake or stream and adversely affect local water quality. Moreover, leaching studies on gasifier ash carried out under different conditions indicate that pH is probably the single most important factor affecting the solubility of trace elements in coal solid wastes, with a general increase in solubility at lower pH levels.[85,86] Thus, in regions with acidic rainfall (which can reach a pH of 3 or lower in some areas in the eastern United States) or in landfills where conditions lead to a lowering of the pH of the interstitial water in the disposed waste, trace element concentrations in gasifier ash leachates may be higher than the levels predicted using the RCRA EP, which uses water acidified to a pH of 5. Since landfill leachates can affect local water quality, leachates from landfill disposal of gasifier waste may be regulated under the Clean Water Act if they are high enough in toxic trace elements to significantly degrade the local water quality. Further field studies are needed before the potential impact from the disposal gasifier ash can be more fully understood. In the meantime, multielement analysis of gasifier waste is an important first step towards the identification of potential problems. Such a screening study can provide a means to identify the elements of most concern and to eliminate those elements with concentrations low enough to pose no significant hazard.

In RTI gasifier ash, six potentially toxic trace elements are found in concentrations greater than their DMEG (health) values. They include arsenic, beryllium, chromium, manganese, nickel, and selenium. Three of these elements, chromium, manganese, and nickel, are found in amounts exceeding the amount input in the feed coals for all gasification runs. The high concentrations of these metals in the gasifier residue are from the erosion of the stainless steel reactor. The enrichment of Cr, Mn, and Ni in bottom ash will probably not occur to as great an extent in full-scale gasifiers whose reactors are composed of refractory material. However, column leaching tests at Oak Ridge National Laboratory (ORNL) on gasifier wastes from various pilot scale processes indicated that pulses of high concentrations of nickel can occur in the leachate during the initial stages of leaching of certain gasifier solid wastes.[83] This suggests that under certain conditions nickel could be a problem during the landfill disposal of gasifier wastes. Conversely, ORNL column leaching studies indicate that chromium is well fixed in gasifier ash and does not leach appreciably.[83]

Other elements whose concentrations exceed DMEG (health) values for solid waste in RTI gasifier ash include arsenic (in 15 out of 16 runs analyzed), beryllium (in 18 out of 20 runs analyzed), and selenium (in 1 out of 21 runs). Lead concentrations approach but do not quite reach the DMEG values. These four elements may be listed as elements of potential concern in gasifier ash on the basis of trace element analyses of RTI gasifier ash. Adding nickel on the basis of the ORNL studies and cadmium, which can reach high concentrations in certain U.S. coals and therefore has been selected as an element of potential concern,[10] brings the number of elements of potential concern in gasifier ash to six. Although these six elements are probably not present in gasifier ash in high enough concentrations to make the waste hazardous as defined by RCRA, environmental problems could conceivably result from the disposal of the gasifier ash, depending on disposal practice and the geochemical and hydrological conditions at the disposal site.

7.0 CONCLUSIONS

Significant conclusions from this study are as follows:

1. Efficient fixed-bed gasification of caking coals presents problems because of the tendency of these coals to agglomerate in the gasifier leading to poor gasification rates and heat transfer characteristics.

2. Glass capillary gas chromatography (GC^2) with specific element detection is a complementary analytical technique to gas chromatography/mass spectrometry (GC/MS) for characterization of complex coal gasifier tar samples. Identification and quantitation of high molecular weight sulfur heterocyclics and primary aromatic amines is difficult because they are present at very low concentrations ($\sim$ ppm) in an extremely complex tar matrix.

3. The most significant coal gasification effluent stream from an environmental standpoint is aqueous condensate, followed by tar, product gas, and finally by ash. However, on an equivalent weight basis, the tar stream is more toxic and mutagenic than aqueous condensate based on cytotoxicity and bioassay tests. Polycyclic aromatic hydrocarbons (PAHs) and tar bases are the most mutagenic among the various tar fractions. Coal pyrolysis and gasification at higher temperatures (as in continuous coal feed versus batch feed) leads to reduced tar mutagenicity. The ash stream is very likely nonhazardous under the Resource Conservation and Recovery Act (RCRA) extraction procedure.

4. The most environmentally significant product gas constituents are carbon monoxide, benzene, hydrogen sulfide, and carbonyl sulfide. The product gas represents a "well-known" hazard in the chemical industry, namely that the product (carbon monoxide) that one is trying to maximize contributes the greatest hazards. The environmentally significant aqueous condensate constituents include phenol/cresols/xylenols (PCX), ammonia, sulfides, thiocyanates, cyanide, arsenic, and chlorides. The environmentally significant tar constituents include various PAHs (especially dibenzo(a,h) anthracene, benzo(a)pyrene, and benzo(a)anthracene), PCX, and arsenic. The environmentally significant ash elements include arsenic, nickel, beryllium, and selenium.

5. The RTI laboratory gasifier produced pollutant and total stream data which compared very favorably to those reported in literature for larger-scale gasifiers. Thus, a laboratory gasifier can simulate large-scale gasifiers and serve as a model for studying problems associated with large-scale gasifiers in a cost-effective manner.

6. Coal liquefaction processes produce liquid and solid effluent streams which are qualitatively similar to gasification aqueous condensate, tar, and ash. Combustion of coal produces, in general, far lower quantities of PAHs compared to gasification of coal on a unit coal basis. Coke plant wastewater is qualitatively similar to coal gasification aqueous condensate and pollutant concentrations in the two are within one order of magnitude.

7. The 95 percent confidence intervals for concentration and production of significant pollutants under a variety of gasification conditions (including coal type, temperature, pressure, coal particle size, etc.) are well within one order of magnitude except for sulfides and some trace elements. A major factor probably is the coal type for sulfur compound production since as much as an order of magnitude or greater variation can occur in the amount of sulfur present in the coal itself.

EPA-287 (Cin.)
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GLOSSARY

AA -- Atomic Absorption Spectrophotometry

CHO -- Chinese Hamster Ovary

CP -- Control Priority

DMEG -- Discharge Multimedia Environmental Goal (health)

DOE -- Department of Energy

DS -- Discharge Severity (health)

EP -- Extraction Procedure under RCRA

EPA -- Environmental Protection Agency

FID -- Flame Ionization Detection/Detector

FPD -- Flame Photometric Detection/Detector

GC -- Gas Chromatography/Chromatograph

GC^2 -- Glass Capillary Gas Chromatography/Chromatograph

GC-TC -- Gas Chromatography-Thermal Conductivity Detection/Detector

GC-MS -- Gas Chromatography-Mass Spectrometry/Spectrometer

GFETC -- Grand Forks Energy Technology Center

HPLC -- High Performance Liquid Chromatography/Chromatograph

ICR -- Industrial Control Remote

MEG -- Multimedia Environmental Goal

METC -- Morgantown Energy Technology Center

NAA -- Neutron Activation Analysis

NIOSH -- National Institute for Occupational Safety and Health

NIPDWS -- National Interim Primary Drinking Water Standards

PAH -- Polycyclic Aromatic Hydrocarbon

PCX -- Phenol, Cresols, and Xylenols

PDU -- Process Development Unit

PF -- Production Factor

PNA -- Polynuclear Aromatic Hydrocarbon (A synonym for PAH)

RCRA -- Resource Conservation and Recovery Act

EPA-287 (Cin.)
(4-79)

RTI -- Research Triangle Institute

SRC -- Solvent Refined Coal Process

TKN -- Total Kjeldahl Nitrogen

UV -- Ultraviolet Detection for HPLC

XAD-2^{R} -- A polymeric sorbent made of styrene and divinylbenzene. A Rohn and Haas trade name.